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DESIGN FOR FLEXIBILITY IN THE FOREST BIOREFINERY SUPPLY CHAIN

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RÉSUMÉ

Le climat d’affaires de industrie papetière nord américaine et européenne change présentement. La baisse de la demande, la volatilité des prix, l’augmentation de la compétition pour l’accès aux matières premières et le contrôle du marché, ainsi que des couts énergétiques passablement élevés poussent les entreprises forestières à rechercher de nouveaux modèles d’affaires afin d’être plus compétitives sur le long terme.

Une des alternatives pour ces entreprises est de se tourner vers le secteur émergent de la bioéconomie et du bioraffinage. Possédant déjà un système d’utilité, un réseau d’approvisionnement de matières premières, un réseau de distribution de produits ainsi qu’un savoir-faire technique ouvrant la porte à de nombreuses possibilités d’intégration massique et énergétique, l’industrie forestière possède plusieurs avantages compétitifs pouvant améliorer la performance économique de l’implantation du bioraffinage.

Plusieurs stratégies différentes peuvent être adoptées pour implanter des activités de bioraffinage au sein d’une entreprise. Par contre, en raison des risques technologiques et des risques de marché associés aux nouveaux procédés et produits, et le manque en capital des entreprises forestières, l’implantation du bioraffinage devrait être effectuée par phase. Des outils d’analyse appropriés sont toutefois requis afin d’identifier les stratégies possibles et les phases d’implantation.

Puisque la chaine logistique (SC) d’une entreprise est critique pour la compétitivité à long terme des bioraffineries, un outil d’analyse de la SC peut donc jouer un rôle clé pour une transformation d’entreprise réussie. Une analyse de la SC calcule le bénéfice pour l’ensemble de la chaine logistique et prend en compte les différents contributeurs de couts qui sont typiquement ignorés dans les analyses économiques, tel que les couts d’inventaire, de transition, etc. Elle peut aussi être utilisée pour prendre en considération la volatilité du marché, et détermine comment la flexibilité inhérente d’un système de production peut être exploitée pour atténuer les risques et maximiser le profit. À cet effet, une analyse de la SC peut aussi être utilisée pour cibler le niveau de flexibilité souhaité d’un système afin d’atténuer les risques de volatilité du marché. De plus, cette analyse offre une meilleure compréhension des couts et de la rentabilité d’une stratégie d’implantation donnée. Ainsi, une analyse de la SC peut être utilisée à deux fins différentes :

- Pour la prise de décision au niveau de conception, et plus précisément, pour cibler le niveau de flexibilité d'un procédé de fabrication,
- Pour comparer différentes stratégies pouvant être poursuivies par une entreprise, en évaluant leur performance selon différentes conditions de marché.

L'objectif de cette recherche est d'illustrer une telle méthodologie de conception, soit une méthodologie qui cible un niveau de flexibilité manufacturière préférable à avoir, qui aide à concevoir le réseau de la SC, et qui permet d'évaluer différentes stratégies de bioraffinage pour transformer une entreprise forestière. Cette méthodologie est démontrée en utilisant une étude de cas qui inclut deux options de produits/procédé, dont des procédés thermochimiques et biochimiques, et plusieurs stratégies d'implantation à implanter au fil du temps.

Le point d'ancrage de cette méthodologie est basé sur les principes de gestion de la chaine logistique centrée sur les marges. Plutôt que d'appliquer une approche traditionnelle centrée sur la production, où la gestion de la capacité des équipements et la minimisation des couts de production prime, une approche centrée sur les marges vise plutôt à maximiser le profit. Pour ce faire, tous les couts encourus au long de la SC doivent être considérés de façon intégrée. De même, le potentiel de flexibilité au sein de la SC, particulièrement au niveau de la production, doit être exploité pour maximiser le profit.

Une formulation mathématique d'optimisation est développée pour représenter une telle mentalité. Selon cette dernière, une méthodologie de conception est proposée afin d'aider le processus de prise de décision stratégique reliée au design de la chaine logistique du bioraffinage. Cette méthodologie est alimentée par d'autres méthodologies qui identifient un ensemble d'options de procédés/produits prometteurs. Elle comprend quatre étapes principales :

1. La définition des alternatives de procédés représentant différents potentiels de flexibilité,
2. La définition d'options de réseau de SC, en tenant compte des caractéristiques des alternatives de procédés, de même que les politiques, les forces et les faiblesses de l'entreprise étudiant ces alternatives procédés/produits,
3. Le ciblage d'un degré de flexibilité manufacturière et d'un réseau de SC associé,
4. L'analyse de stratégies d'implantation des alternatives procédés/produits retenues

Un ensemble d'indicateurs de performance représentant la rentabilité de la SC, la robustesse et la flexibilité des différentes options de bioraffinage est utilisé pour évaluer la performance de stratégies de bioraffinage selon différents scénarios de marchés.

Les résultats montrent que lorsque la flexibilité d'un système est améliorée, le profit augmente. Cependant, cela ne mène pas nécessairement à une amélioration de la rentabilité. Pour que la rentabilité d'un système flexible augmente, les investissements supplémentaires déboursés pour augmenter le degré de flexibilité doivent être compensés par une amélioration au niveau des profits. Ainsi, pour certains cas, la rentabilité augmente avec la flexibilité du procédé, et dans certains cas non. De plus, la robustesse d'une option est directement liée à sa flexibilité. Plus le degré de flexibilité augmente, plus le système devient robuste envers la volatilité du marché.

De même, les résultats montrent l'importance de l'analyse de la SC lors de la prise de décision reliée à la conception. Ils illustrent le fait qu'un changement dans le degré de flexibilité manufacturière d'un procédé affecte directement les opportunités de l'entreprise. Ainsi, des stratégies de marché et des degrés de flexibilité différents impliquent une configuration de réseau de SC et une stratégie de gestion spécifiques. Il devrait donc y avoir une intégration entre la conception de procédés et la conception du réseau de la SC.

Il est aussi montré que les produits chimiques à valeur ajoutée sont prometteurs pour le succès futur du bioraffinage. Les options de procédés fabriquant ces derniers obtiennent une rentabilité en termes de taux de retour interne considérablement plus élevée que les options fabriquant des produits de commodités.

ABSTRACT

The pulp and paper industry business environment in North-America and Europe is changing. Declining and volatile product price and demand, increased competition for feedstock and market share, growing competition from global low-cost producers and considerably high energy cost are driving companies to seek alternative business models to be competitive over the longer term. One alternative is to enter the bio-energy and biorefinery sectors that have been emerging in recent years. Having the required utility systems in place and the engineering know-how, existing feedstock supply chain networks and product delivery systems as well as the potential for mass and/or energy integration between existing processes and new processes imply competitive advantages for the forestry companies to improve their economic performance via implementing biorefinery.

Many different strategies can be pursued for implementing the biorefinery. Due to a lack of capital for implementing such strategies, technological risks and product market immaturities, the implementation should be executed in a phase-wise manner. Proper analysis tools are required to identify feasible strategies and their implementation phases.

The design and management of supply chain (SC) is critical for the long-term competitive advantage of companies who would like to implement the biorefinery. In this regard, SC analysis can be used to evaluate the potential SC performance of different biorefinery strategies. It calculates the profit across the entire SC and accounts for cost contributors that are typically ignored in economic analyses, e.g. inventory cost, changeover cost, etc. It can also be used to take into consideration market volatility, and determine how the flexibility of the manufacturing system can be exploited to mitigate market risks in order to maximize profit. In this way, SC analysis can be used to target the desired level of flexibility of a manufacturing system needed to mitigate the impact of market price volatility. Moreover, these capabilities provide better insight into the costs and profit incurred by an implemented strategy. Thus, an SC analysis can be used for two different purposes:

- For making design decisions, and more specifically, for targeting the level of flexibility of a system and designing the SC network configuration
- For comparing several strategies by evaluating their performance for different market conditions

The objective of this thesis is to develop a design methodology for targeting the required level of flexibility, designing the SC network configuration, and evaluating different FBR strategies for transforming a forest company. The methodology is demonstrated using a case study that involves two product/process options, including thermochemical and biochemical processes, with several implementation strategies, implemented over the years.

The pivot of this methodology is the margins-based thinking used as an operating policy. It is discussed that, instead of applying the traditional manufacturing-centric approach in production which focuses on capacity management and tries to minimize the costs, the margins-based policy must be implemented, which has the following specifications:

- It maximizes the profit instead of minimizing costs
- It considers all costs incurred by SC activities in an integrated manner and doesn't only focus on production cost
- It exploits the potential for flexibility in the SC, especially in production, to maximize profit

A SC optimization formulation is developed to represent such thinking. Using this formulation, a design methodology is proposed for making strategic decisions related to biorefinery SC design. This methodology is fed by separate methodologies which identify the most promising set of product to produce and technologies to employ. Given that, the methodology involves four major steps:

- Defining process alternatives representing different potentials for flexibility
- Defining SC network alternatives based on the defined process alternatives as well as the policies, advantages and restrictions of the company
- Targeting the level of flexibility of processes and determining its associated SC network
- Analyzing different implementation strategies for the proposed product/processes with their targeted level of flexibility and defined SC network

A set of performance metrics that represents SC profitability, robustness and flexibility is used to evaluate the performance of biorefinery strategies for several market scenarios.

The results show that when the flexibility of a system is enhanced, its profit increases. But this does not necessarily end in profitability improvement. For the profitability of a flexible system to improve, the extra capital cost paid for increasing the level of flexibility must be compensated by the profit improvement. Thus, for some cases profitability increases with flexibility and for some cases it does not. Moreover, robustness has a direct relationship with flexibility. As flexibility increases, the system becomes more robust against market volatility.

The results reveal the importance of SC analysis in making design decisions. They illustrate that changes in the level of flexibility will directly affect the company's opportunities and strategies in the market, and thus, each level of flexibility implies a specific SC network configuration and management strategy. Therefore, there must be integration between process design and SC network design.

It is also shown that added-value chemicals are promising for the long-term success of biorefineries. Their profitability, in terms of internal rate of return (IRR), is considerably higher than that of commodities.

CONDENSÉ EN FRANÇAIS

Depuis quelques années, l'industrie forestière nord-américaine fait face à de nombreux défis, tels qu'une baisse de la demande, une demande volatile, une concurrence globale accrue provenant de producteurs à faible cout, une augmentation de la compétition pour l'accès aux matières premières et pour l'accès au marché, des couts énergétiques passablement élevés, des lois de plus en plus strictes et des attentes élevées de la société en ce qui a trait à l'environnement. À cela s'ajoute le fait que les usines nord-américaines sont vieillissantes et que l'industrie est intensive en termes de capitaux. Le manque de recherche et développement au sein des entreprises forestières ont abouti à un faible niveau d'innovation en termes de développement de produits et de nouvelles stratégies d'affaires. Par conséquent, ces entreprises doivent maintenant rechercher de nouveaux modèles d'affaires afin d'être plus compétitives sur le long terme. D'un autre côté, les entreprises forestières possèdent plusieurs avantages compétitifs pour l'implantation de nouveaux procédés qui amélioreraient leur performance économique. Celles-ci possèdent déjà un système d'utilité, un réseau d'approvisionnement de matières premières, un réseau de distribution de produits ainsi qu'un savoir-faire technique, ouvrant la porte à de nombreuses possibilités d'intégration massique et énergétique.

Une des alternatives pour ces entreprises est de se tourner vers le secteur émergent de la bioéconomie et plus précisément le bioraffinage forestier, une sous-catégorie du bioraffinage qui vise principalement à transformer la biomasse forestière en rétro-installation dans les usines de pâtes et papier existantes. Ainsi, le point de départ pour une entreprise forestière désirant améliorer sa performance économique est de prendre un point de vue stratégique pour cette transformation au bioraffinage, en produisant de nouveaux produits, mais aussi en changeant les façons de faire, compte tenu des avantages compétitifs existants. En d'autres mots, une entreprise forestière désirant améliorer son modèle d'affaire devrait non seulement diversifier ses revenus, mais modifier aussi sa culture d'entreprise.

Plusieurs stratégies différentes peuvent être adoptées pour implanter des activités de bioraffinage au sein d'une entreprise. Par contre, en raison des risques technologiques et des risques de marché associés aux nouveaux procédés et produits, ainsi que le manque de capital des entreprises forestières, l'implantation du bioraffinage devrait être effectuée par phase. Selon cette approche stratégique par phase du bioraffinage forestier, la diversification des revenus serait d’abord accomplie par une « perturbation technologique », où des produits chimiques intermédiaires seraient fabriqués à court terme. Idéalement, à plus long terme, ces intermédiaires seraient transformés en dérivés à valeur ajoutée. D’un autre côté, la culture d’entreprise serait modifiée par « perturbation des affaires », en appliquant de nouvelles politiques de gestion de la chaine logistique et en exploitant la flexibilité manufacturière. Des outils d’analyse appropriés sont toutefois requis afin d’identifier les stratégies possibles et les phases d’implantation. Puisque la chaine logistique (SC) d’une entreprise est critique pour la compétitivité à long terme de bioraffineries, un outil d’analyse de la SC peut donc jouer un rôle clé pour une transformation d’entreprise réussie.

La gestion au sein des entreprises forestières est typiquement centrée sur la capacité des équipements. De ce fait, la rentabilité de la chaine logistique est généralement ignorée. Pour une transformation au bioraffinage, il est important de changer cette mentalité. À court terme, afin d’atténuer les risques reliés à la volatilité du marché, les entreprises devraient implanter des *politiques de gestion de la SC centrée sur les marges* et mieux utiliser la capacité des procédés afin d’avoir une *production flexible*. Or, une analyse de la SC effectue la planification de la production sur différents horizons de temps et identifie les compromis à faire entre la production et l’offre et la demande anticipée. Elle calcule le bénéfice pour l’ensemble de la chaine logistique et prend en compte les différents contributeurs de couts qui sont typiquement ignorés dans les analyses économiques, tel que les couts d’inventaire, de transition, etc. Cette analyse peut donc être utilisée pour prendre en considération la volatilité du marché, et pour déterminer comment la flexibilité inhérente d’un système de production peut être exploitée pour atténuer les risques et maximiser le profit.

À plus long terme, les entreprises devraient fonder leurs décisions stratégiques selon une approche ascendante, c’est-à-dire concevoir la SC de la future bioraffinerie en se basant sur les effets de celle-ci sur les activités au niveau opérationnel. À cet effet, une analyse de la SC peut être utilisée pour cibler le niveau de flexibilité souhaité d’un système afin d’atténuer les risques de volatilité du marché. De plus, cette analyse offre une meilleure compréhension des couts et de la rentabilité d’une stratégie d’implantation donnée. Ainsi, une analyse de la SC peut être utilisée non seulement pour les décisions à court et moyen terme reliées à la gestion de cette dernière, mais aussi pour aider à la prise de décision à plus long terme. Plus précisément, en apportant des informations du niveau opérationnel d'un procédé au niveau de conception, une analyse de la SC peut être utilisée au niveau stratégique de prise de décision pour :

- Cibler le niveau de flexibilité d'un procédé de fabrication
- Concevoir le réseau de la chaine logistique d'une entreprise
- Comparer différentes stratégies pouvant être poursuivies par une entreprise, en évaluant leur performance selon différentes conditions de marché.

Une méthodologie de conception qui inclut une analyse de la SC pouvant refléter les effets des activités opérationnelles futures au stade de la conception, et qui examine comment différentes stratégies d'implantation de bioraffinage performeront à court terme dans des conditions de marché volatiles, pourrait potentiellement aider lors du processus de décision pour la transformation vers le bioraffinage forestier.

L'objectif de cette recherche est d'illustrer une telle méthodologie de conception, soit une méthodologie qui cible un niveau de flexibilité manufacturière préférable à avoir, qui aide à concevoir le réseau de la SC, et qui permet d'évaluer différentes stratégies de bioraffinage pour transformer une entreprise forestière. Cette méthodologie de conception fusionne la conception du réseau de la SC et la conception pour la flexibilité de procédés, et les intègre à des méthodologies existantes de conception du portefeuille de procédés/produits et d'analyses du cycle de vie. Elle utilise un modèle d'optimisation générique de la chaine logistique spécifiquement développé pour le bioraffinage, et qui permet d'évaluer la performance de stratégies au niveau opérationnel. Un ensemble d'indicateurs de performance représentant la rentabilité de la SC, la robustesse et la flexibilité de diverses options de bioraffinage est utilisé pour évaluer la performance de stratégies de bioraffinage selon différents scénarios de marchés, et pour identifier les options prometteuses. Cette méthodologie est démontrée en utilisant une étude de cas qui inclut deux options de procédés/produits, dont des procédés thermochimiques et biochimiques, et plusieurs stratégies d'implantation à implanter au fil du temps.

Cette méthodologie comprend quatre étapes principales :

Lors de la première étape, un ensemble de portefeuilles de produits ainsi qu'un ensemble de procédés technologiques pour fabriquer ces produits sont considérés. La méthodologie pour choisir cet ensemble de procédés/produits n'est pas incluse dans la présente méthodologie. Ensuite, pour chacun des portefeuilles, le système de production est caractérisé en termes de volume de flexibilité et de flexibilité de produits. Quelques alternatives de procédés, représentant chacune un potentiel spécifique de flexibilité, sont ainsi définies à l'aide d'heuristiques d'ingénierie. Les couts d'investissement et d'opération de chaque alternative sont aussi calculés. À noter, le modèle d'optimisation n'est pas encore utilisé à cette étape.

Lors de la seconde étape, quelques options de réseau de SC sont définies pour chacun des portefeuilles procédés/produits. Pour ce faire, les caractéristiques des alternatives de procédés, de même que les politiques, les forces et les faiblesses de l'entreprise doivent être considérés. L'investissement requis pour chacune des options de réseau de SC est aussi calculé. À la fin de cette étape, les combinaisons de procédés sont jumelées aux diverses options de réseau de SC.

Lors de la troisième étape, différentes fenêtres d'opération sont définies pour chaque alternative. Le modèle d'optimisation de la SC est exécuté pour chacune de ces fenêtres d'opération selon divers scénarios de marché représentant différents niveaux de volatilité de marché en termes de prix et de demande. Un profit est donc calculé pour chaque fenêtre d'opération. La meilleure fenêtre d'opération pour chacune des options de procédés, montrant le degré de flexibilité adéquat, peut alors être déterminée. Les trois indicateurs de performances utilisés pour déterminer les fenêtres d'opération sont la rentabilité de la SC, la robustesse de l'option ainsi que sa flexibilité

Lors de la dernière étape, un nombre restreint de stratégies d'implantation est défini pour chacun des portfolios, selon leurs caractéristiques respectives, leur flexibilité ciblée et selon le contexte de l'entreprise. Le modèle d'optimisation de la SC est utilisé à cette étape pour évaluer la performance de chacune des stratégies au cours de leur durée de vie et selon différents scénarios de marché. Une analyse Monte Carlo est également effectuée pour donner un meilleur aperçu de la robustesse de chacune des stratégies.

Les principales contributions de cette thèse sont :

1. Une méthodologie systématique de conception pour la conception de la chaine logistique de bioraffineries
   - Qui sépare la conception de la SC en un ciblage du degré de flexibilité manufacturière adéquat et la conception du réseau de la SC,
   - Qui offre le potentiel d'être intégrée à des méthodologies de définition du portefeuille de produits et à des analyses technico-économiques, et qui peut fournir des

informations et critères pertinents pour d’autres analyses telles que l’analyse du cycle de vie et l’analyse multicritère de décision (MCDM),

- Et qui apporte des considérations opérationnelles au niveau stratégique de prise de décision afin d’analyser les effets d’une conception sur l’opération.
- Cette méthodologie prétend être efficace pour des études de cas, des projets concrets et industriels. En fait, un point de vue de l’entreprise est considéré afin de fournir un cadre systématique de conception qui n’est pas trop compliqué, mais qui permet à la fois de résoudre des problèmes industriels en utilisant les avancées récentes en gestion de la SC et en ingénierie des systèmes.

2. Une concrétisation du concept de planification basée sur les marges dans le contexte du bioraffinage forestier.
    - La valeur de la planification basée sur les marges pour l’amélioration de la rentabilité de bioraffineries a été comparée à l’approche plus traditionnelle centrée sur la production dans différentes conditions de marché, et ce pour des produits de commodité et à valeur ajoutée.
3. La création d’indicateurs de performance de la chaine logistique, notamment
    - Un critère de rentabilité de la SC considérant les divers contributeurs de couts qui offre une meilleure représentation des couts du système comparativement aux indicateurs économiques habituels qui mettent plutôt l’accent sur les couts reliés aux procédés,
    - Un critère de robustesse simple qui mesure l’écart entre le profit dans le pire des cas et le profit du cas de base,
    - Un critère de flexibilité qui quantifie la flexibilité en termes de volume et de produits, montrant la déviation du volume de production par rapport au taux nominal de production de tous les produits,
    - Un paramètre de type valeur à risque conditionnelle (CVAR) qui peut être utilisé pour analyser les risques associés à des stratégies de ventes, comme par exemple, la décision d’allouer une partie de la capacité de production aux ventes au comptant, et la décision du pourcentage de contrats devant être acceptés.
    - Tous ces paramètres peuvent être utilisés simultanément afin d’analyser la performance d’une SC, et pour déterminer le degré de flexibilité manufacturière et la

configuration de réseau de SC offrant la meilleure performance au niveau opérationnel.

4. Une méthode permettant le ciblage d'un degré de flexibilité manufacturière adéquat pour atténuer les risques du marché
    - Qui considère divers couts et aspects de la SC, incluant notamment l'approvisionnement, l'inventaire et le transport, et non seulement les couts et considérations du procédé.
5. L'application d'une approche simplifiée basée sur les scénarios pour la conception de la chaine logistique du bioraffinage forestier, qui vise à identifier les options réalistes qui semblent meilleures que d'autres.

Les aspects suivants présentent quelques opportunités de recherche

- Cette méthodologie est liée et alimentés par d'autres méthodologies de définition de portefeuille de produits et d'études technico-économiques. Elle offre aussi quelques critères et indicateurs de performance qui pourraient être utilisés dans un cadre d'analyse multicritères de décision (MCDM). Ainsi, une opportunité de recherche consiste à l'intégration cette méthodologie à des analyses du cycle de vie environnemental et social afin de prendre en compte les aspects de développement durable liés au bioraffinage.
- La méthodologie proposée ne vise pas à concevoir la flexibilité de procédés. Elle aborde plutôt une étape précédant celle-ci, le ciblage du degré de flexibilité. Ainsi, une opportunité de recherche serait de justement concevoir ce degré de flexibilité ciblé où l'opérabilité et de contrôlabilité devraient être considérés pour 1) vérifier que le procédé est opérable à l'intérieur de la fenêtre de flexibilité, et 2) fournir une estimation plus précise des délais de transition entre façons d'opérer.
- Une modification de la formulation mathématique afin de représenter l'incertitude selon une approche stochastique à deux niveaux. Les décisions reliées à la conception peuvent être déterminées en utilisant ce genre de formulation plutôt que par heuristiques, comme il l'a été effectué dans cette thèse.

Une autre opportunité de recherche consiste à développer davantage la formulation mathématique du modèle de modèle de planification opérationnelle pour créer un modèle hybride de planification et de conception de procédé.

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LIST OF ABBREVIATIONS

CCF	Cumulative Net Cash Flow
CVAR	Conditional Value at Risk
FBR	Forest Biorefinry
FTL	Fischer-Tropsch Liquids
GTL	Gas-to-Liquid
HFTL	Heavy Fischer-Tropsch Liquids
HRSG	Heat Recovery Steam Generator
IRR	Internal Rate of Return
JF	Jet Fuel
LA	Lactic Acid
LCA	Life Cycle Analysis
LFTL	Light Fischer-Tropsch Liquids
LP	Linear Programming
MA	Malic Acid
MCDM	Multi-Criteria Decision Making
MF	Metric of flexibility
MFTL	Medium Fischer-Tropsch Liquids
MILP	Mixed Integer Linear Programming
MINLP	Mixed Integer Non-Linear Programming
MR	Metric of Robustness
NLP	Non-linear Programming
NPV	Net Present Value
OA	Contractual Order Acceptance Percentage

PLPW	Pressurized Low Polarity Water
P&P	Pulp and Paper
ROI	Return on Investment
SA	Succinic Acid
SC	Supply Chain

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INTRODUCTION

Problem statement

Over the past few years, forestry industry in North America have been facing significant challenges related to declining and volatile market demand, growing competition from global low-cost producers, increasing competition for feedstock and market share, considerably high energy cost, strict regulations and high environmental expectations from the public. We must add to these the capital intensiveness of the industry and its aging mills and equipment. Lack of R&D activities in forestry companies have resulted in a low level of innovation in terms of developing new products and new ways of doing business. Hence, forestry companies are driven to seek alternative business models to be competitive over the longer term. On the other hand, having the required utility systems in place and the engineering know-how, existing feedstock supply chain networks and product delivery systems, as well as the potential for mass and/or energy integration between existing processes and new processes imply competitive advantages for the forestry companies to improve their economic performance. In other words, the aforementioned advantages provide the opportunity of implementing new processes along with the existing processes.

One alternative for forestry companies is to enter the bio-energy and biorefinery sectors that have been emerging in recent years. More specifically, the forest biorefinery (FBR), i.e. a category of biorefineries which primarily aims to process forest biomass as raw material typically in retrofit to existing pulp and paper (P&P) mills, is viewed as a strong option. Therefore, the starting point for a forestry company willing to enhance its economic performance is to take a strategic view of transforming its core business to FBR by producing new products and by changing the way of doing business, given its competitive advantages. In other words, for a forestry company to improve its business model in the current market situation, it not only should diversify its revenue, but also must change its current manufacturing culture and its thinking behind the way of doing business.

Many different strategies can be pursued for implementing the biorefinery by a forestry company. However, due to the lack of capital for implementing such strategies, technological risks and product market immaturities, the implementation should be executed in a phase-wise manner. In this strategic phased approach for implementing the FBR, revenue diversification will be achieved by means of “technology disruption” by producing building-block chemicals in the short term, and ideally, in the longer term, by further increasing revenues by producing added-value derivatives. On the other side, manufacturing culture will be changed via “business disruption,” through applying novel supply chain operating policies and exploiting production flexibility. Proper analysis tools are required to identify feasible strategies and their implementation phases. Supply chain (SC) design and management are critical for the long-term competitive advantage of companies which would like to implement the biorefinery, and thus, an SC analysis tool can play a key role for a successful transformation.

For revenue diversification purposes, several product/process options are available for a company, considering its existing condition and characteristics, which can be implemented through phases and an SC analysis can be used to evaluate the potential SC performance of these different options over the long run.

SC analysis is of more importance for the business disruption purposes. In the forestry companies, the management focus is on capacity management and the profitability of the entire SC is generally ignored. It is important to change this way of thinking. On one side, in the short term, to mitigate the risks of market volatility, companies should focus on improving their margins by implementing a *margins-based SC operating policy* and better exploiting the process capability for *flexible production*. SC analysis carries out product planning over different time horizons and identifies trade-offs between product orders and anticipated supply and demand. It calculates the profit across the entire SC and accounts for cost contributors that are typically ignored in economic analyses, e.g. inventory cost, changeover cost, etc. It can also be used to take into consideration market volatility, and to determine how the flexibility of the manufacturing system can be exploited to mitigate market risks in order to maximize profit. On the other side, over the long term, companies should base their strategic decisions on a bottom-up approach, i.e. to design the SC based on the effect of the design on operational activities. As mentioned earlier, SC analysis can help identifying how the flexibility of a system must be exploited to maximize the profit in a volatile market. Using this capability, SC analysis can be used to target the desired level of flexibility of a manufacturing system needed to mitigate the risk of market volatility. Moreover, these capabilities provide better insight into the costs and profit incurred by an implemented strategy. Thus, an SC analysis can be used, not only for making mid- and short-term decisions related to the management of the SC, but also for making long-term design decisions. More specifically, by bringing up the operational issues of a manufacturing system to the design level, SC analysis can be employed at the strategic level for:

- Targeting the level of flexibility of a manufacturing system
- Designing the SC network of a company
- Comparing several strategies, that can be pursued by a company, by evaluating their performance for different market conditions

A design methodology including an SC analysis that can reflect the effect of operational activities at the design stage, and in this way, examines how each FBR implementation strategy will perform in volatile market conditions, can potentially better serve the decision making process for the FBR. The goal of this research is therefore to illustrate a design methodology for evaluating different FBR strategies for transforming a forestry company. This design methodology incorporates the SC network design into the design for process flexibility, and integrates them with the existing methodologies of product/process portfolio definition and life cycle analysis (LCA). The methodology uses a generic operational SC optimization model developed for biorefineries that can evaluate the performance of strategies at the operational level. The methodology is demonstrated using a case study that involves two product/process options, including thermochemical and biochemical processes, with several implementation strategies, implemented over the years. A set of performance metrics representing SC profitability, robustness and flexibility is used to evaluate the performance of biorefinery strategies for several market scenarios and to identify the promising ones.

Objectives

As mentioned, the ultimate goal of this thesis is to present a SC design methodology which evaluates different biorefinery strategies based on their operational SC performance. Each strategy consists of a set of product/process portfolios defined by separate methodologies. The goal is to target the flexibility of processes, to design the SC network configuration, and to propose an implementation strategy. Before getting to these design activities, the appropriate operating policy for the FBR must be identified. Then, relevant performance metrics must be developed to help designing a flexible system against a volatile market. Finally, the strategic and design activities, i.e. targeting level of flexibility, SC network design, and identifying implementation strategy can be carried out.Based on that, the main hypothesis of this work entitled “Design for flexibility in the forest biorefinery supply chain” was formulated:

> *A systematic SC design methodology can be developed for the evaluation of FBR product-process strategies that exploits margins-based policy and manufacturing flexibility, and can assess the viability of phased implementation for forest company transformation*

This can be divided into four sub-hypotheses:

- *A margins-based SC operating policy is essential for managing the FBR product portfolio in order to enhance the likelihood of success by internalizing risk due to product price volatility*
- *Simple metrics can be calculated at the early-design stage to illustrate the trade-off between SC robustness and profitability with increasing manufacturing flexibility*
- *The flexibility of FBR processes can be targeted through SC analysis using a tactical/operational SC model for a given product portfolio*
- *FBR SC strategic-level design should be evaluated using a scenario-based approach, that considers the impact of SC design decisions on operational-level profit*

The problem statement and the hypothesis call for the development of a systematic methodology that exploits the margins-based operating policy, and by developing relevant SC performance metrics, targets the level of flexibility and designs the SC network in order to mitigate the risks of market volatility. Furthermore, the methodology is ultimately suited to evaluate FBR options to be implemented through phased strategies, and to identify the best strategy. As such, the formulation of the methodology was guided by the following main objective:

> *To illustrate an overall SC design methodology at the operational, tactical and strategic levels, and to calculate metrics for evaluating dissimilar transformational biorefinery strategies, using several FBR case-study examples involving commodity and added-value products*

The accomplishment of the main objective was tied to following sub-objectives:

- *To compare margins-based operating policy with the manufacturing-centric approach using an operational SC model for different product-process FBR strategies*

- *To identify a practical robustness metric that is a function of manufacturing flexibility, and can be calculated at the early-design stage using the tactical/operational SC model*
- *To evaluate the trade-off between cost of manufacturing flexibility and SC profit under different conditions of market price and demand volatility, using a margins-based SC policy*
- *To assess pertinent SC design scenarios associated with FBR strategies/partnerships by evaluating the effect of SC design decisions on operational-level profit*

Thesis organization

This thesis is organized as follows: In chapter 1, the relevant literature is reviewed in order to identify the gaps in the body of knowledge. Chapter 2 presents the supply chain mathematical formulation, the methodology developed in this thesis, and the case study to which the methodology is applied. Chapter 3 synthesizes the results obtained in the process of demonstrating the methodology. In chapter 4, overall conclusions are given, followed by chapter 5 which presents the contributions to knowledge and recommendations for future work.

In Appendices A to E the articles that were published in or submitted to peer-reviewed scientific journals are given. Other complementary papers are in Appendices F to J. The link between the hypotheses and major publications are illustrated in Figure 0-1.

	Contribution	Publication
Appendix A	**Methodology**	**Integrating product portfolio design and supply chain design for the forest biorefinery** (Computers & Chemical Engineering)
Appendix B	**Performance metrics** 2nd hypo.	**Metrics for evaluating the biorefinery supply chain performance** (Computers & Chemical Engineering)
Appendix C	**Targeting flexibility** 3rd hypo.	**Incorporating flexibility design into supply chain design for the forest biorefinery** (JFOR)
Appendix D	**Scenario-based SC design** 4th hypo.	**Scenario-based strategic supply chain design and analysis for the forest biorefinery** (Production Economics)
Appendix E	**Wrap up** **Phased approach**	**A systematic biorefinery supply chain design methodology incorporating a value-chain perspective** (PPI)

Figure 0-1 Linkage between hypothese and publications

CHAPTER 1 LITERATURE REVIEW

1.1 Supply chain design and management

Several definitions have been proposed for SC. According to Chopra, SC means all stages that are involved, directly or indirectly, in fulfilling a customer request. It consists of the suppliers and manufacturers, transporters, warehouses, retailers and finally customers (Chopra, 2007). An SC is a network of facilities and distribution mechanisms in which material procurement, material transformation to intermediates and final products, and distribution of these products to customers are performed (Papageorgiou, 2009). As stated by Beamon, an SC can be defined as an integrated network in which a number of business entities including suppliers, manufacturers, distributors, and retailers work together in order to: (1) acquire raw materials, (2) convert raw materials into specified final products, and (3) deliver final products to retailers/customers. In an SC, materials flow from suppliers to the customers, while the information flow backward (Beamon, 1998).

SC-related problems are classified into three categories: Strategic design, which involves long-term decisions, tactical planning, which deal with mid-term decisions, and operational scheduling, which address short-term decisions (chopra, 2007). A similar classification is introduced by Shah: (1) supply chain infrastructure (network) design; (2) supply chain analysis and policy formulation; (3) supply chain planning and scheduling (Shah, 2005). The first two categories include relatively infrequent activities that are defined and implemented in order to establish the best way to configure and manage the SC network. The last one comprises decision making about how to operate the SC network to respond in the best way to the external conditions encountered by the SC. Papageorgiou included SC control, i.e. SC real-time management, in these classifications (Papageorgiou, 2009). In general, the strategic level dealing with long-term decisions is referred to as SC design, while planning, scheduling and control levels dealing with mid- to short-term activities are referred to as SC management.

1.1.1 Supply chain levels

1.1.1.1 Supply chain strategic design

At the strategic level, decisions are made about how to structure the SC in long term. At this level, the structure of the SC network, final products, processes and technologies, number, location and capacity of plants and warehouses, raw material resources and procurement strategies, transportation modes and type of information system to be employed have to be determined (chopra, 2007). Significant changes to existing facilities, e.g. expansion, contraction or closure, sourcing decisions, e.g. what suppliers and supply base to use for each facility, allocation decisions, e.g. what products should be produced at each production facility, which markets should be served by which plants/warehouses, etc. are different types of decisions that must be made at the strategic level (Shah, 2005).

At this level, the decision variables are generally classified into two categories; binary variables, concerning the “Yes/No” decisions, e.g. whether a process must be installed or not, and continuous variables, e.g. rate of production, rate of flow of material from plants to warehouses, etc (Tsiakis, shah, & Pantelides, 2001). The objective at this level is to maximize profit or minimize the total annualized cost of the network, taking into consideration both infrastructure and operating costs. More specifically, the major goals at the strategic level include minimization of costs, delivery delays, inventories, and investments, or maximization of deliveries, profit, return on investment, customer service level, and production. The infrastructure costs are related to the costs incurred by design and construction of manufacturing facilities and other facilities establishment, i.e. warehouses and distribution centers. On the other hand, operating costs are related to the rate of production of each product, cost of change-over as lost products, material handling costs at warehouses and distribution centers and transportation costs caused by transporting material between any nodes in the supply chain network (Tsiakis, shah, & Pantelides, 2001).

Early research in this field was started by focusing on location-allocation problems. Geoffrion and Graves (1974) develop a model for designing distribution systems with optimal location of the distribution facilities between plants and customers. This problem is evolved to facility selection, equipment location and utilization, and product manufacturing and distribution

(Brown, Graves, & Honczarenko, 1987). In the next decades, more complicated models are introduced for the design of multi-product multi-echelon SC networks, integrating components associated with optimal product portfolio, production and long-term capacity planning, facility location, product transportation, and distribution (Pirkul & Jayaraman, 1998), (Tsiakis, shah, & Pantelides, 2001; Papageorgiou, Rotstein, & Shah, 2001; Sousa, Shah, & Papageorgiou, 2008; Guillen, Mele, Bagajewicz, Espuna, & Puigjaner, 2005). Tsiakis and Papageorgiou (2008) incorporate the out-sourcing of production as a business decision whenever the organisation cannot satisfy the demand into classical product-site location problems.

A further improvement to these problems is made by developing methodologies and models to design the production-distribution network of divergent process industry companies in a multinational context (Mohamed, 1999; Martel, Vila, & Beauregard, 2006; Naraharisetti, Karimi, & Srinivasan, 2008a). An important issue to address in multinational problems is to incorporate the effects of changing and high inflation rates and changing exchange rates under which a facility has to operate in a host country.

In recent years, integrating SC design models with other analysis tools has got attention. For instance, reducing the environmental impacts of industries' end products has been addressed by researchers. Frota Neto, Bloemhof-Ruwaard, van Nunen, and van Heck (2008) show how the environmental concerns can be entered the network design problems by introducing environmental impact parameters. Companies trying to diminish the environmental impact of their logistic networks should look for good trade-offs between environmental impact and costs. Guillén-Gosálbez & Grossmann (2010) addressed the optimal design and planning of sustainable chemical supply chains using a bi-criterion stochastic non-convex mixed-integer nonlinear program which accounts for both net present value (NPV), and environmental performance of the network through Eco-indicator 99, which included recent advances made in life cycle assessment. Another example is the simultaneous consideration of economic performance and responsiveness of the multi-site multi-echelon SC networks which is addressed by You and Grossmann (2008).

Overall, SC design problems have evolved considerably and the evolution of optimization models help researchers addressing more complicated problems. However, as stated by Papageorgiou (2009), there are still some issues to be investigated such as (1) level of detail in the process representation, (2) potential integration with process modelling tools, (3) dealing efficiently with size of problem, (4) dealing with model nonlinearities, and (5) inclusion of performance measures other than cost/profit.

1.1.1.2 Supply chain tactical planning

At the tactical planning level, the operating policies for short term must be defined subject to the constraints established by the decisions made at the strategic level, and by forecasting the market conditions, the processes should be planned to fulfil the customers' requests. In comparison with the strategic level, at the planning level decisions are made for shorter period, e.g. months or weeks (chopra, 2007). Decisions made at this level determine the markets that will be supplied from a special location, the type of products that must be produced in a specific location, the amount of each product that must be produced, the allocations of resources to the various product families, the replenishment and inventory policies that should be followed, and the amount of material that must be transported between facilities or to the market (Kreipl & Pinedo, 2004). The goal of this level is to maximize the mid-term profit and to minimize the total cost including production costs, sequence dependant changeover cost at the production stage, storage costs, transportation costs, tardiness costs, non-delivery costs, handling costs, costs for increases in resource capacities, and costs for increases in storage capacities (Kreipl & Pinedo, 2004).

Kallrath (2002a) presented a comprehensive review on planning and scheduling in the process industry. Kreipl and Pinedo (2004) gave an overview of the theory and practice of planning models in SCs. SC planning studies got attention in 90s. Several multi-period mathematical models for process industry supply chains are proposed in this decade, including a production/distribution planning model by Wilkinson, Cortier, Shah, and Pantelides (1996), a mathematical model designed to improve efficiency and responsiveness in a supply chain by Voudouris (1996), and a multi-period linear programming model for planning of single-stage continuous processing lines by McDonald and Karimi (1997). In 2000s, the research in this field gets diverse. Timpe and Kallrath (2000) propose a formulation which covers the relevant features required for the complete SC management of a multi-site production network. Their model combines aspects related to production, distribution and marketing, includes production sites and sales points, and finally addresses some aspects such as how to define the capacity of a multi-site, multi-product production network, or how to approach complex planning problems. Jin-

Kwang, Grossmann, and Park (2000) introduce a multiperiod optimization model for continuous process networks for making operational decisions over short time horizons from one week to one month, considering sales, intermittent deliveries, production shortfalls, delivery delays, inventory profiles and job changeovers. Pinto, Joly, and Moro (2000) describe a refinery planning model with non-linear process models and blending relations. Perea, Grossmann, Ydstie, and Tahmassebi (2001) address the dynamic nature of SC management as well as the design of systematic decision-making processes for SC by proposing a dynamic framework to model SC at the planning level based on the application of ideas from process dynamics and control. The framework models the flow of information and material within the SC, and employs them to capture its dynamic behaviour. Jackson and Grossmann (2003) propose a multi-period model to address the production planning and product distribution of several continuous multi-product plants that are located in different sites and supply different markets. The proposed model reflects and predicts the production behaviour of each plant and determines each plant's product distribution. The only major simplification is that changeovers are neglected. Neiro and Pinto (2004) develop a general framework for modeling petroleum SCs for planning purposes. Decisions include selection of oil types and their transportation plan, production levels respecting quality constraints as well as operating variables of processing units at refineries and product distribution plan and inventory management along the planning horizon.

An evolution in this category was the inclusion of logistics operations in the production planning of processes. Amaro and Barbosa-Povoa (2008) focused on this issue.

1.1.1.3 Supply chain operational scheduling

At the operational level, the operational policies are implemented within the fixed SC structure, which was made at the strategic level, and according to the policies which were defined at the planning level, in order to either maximize the profit or minimize the total costs. The time period is shorter, e.g. weeks or days. On this time scale the decisions are made regarding the individual customer orders by allocating them to inventory and production, setting date for the order fulfillment, arranging schedules for warehousing and then transporting the end product to customers (chopra, 2007). In each detailed scheduling problem the scope is considerably narrower with regard to time as well as space, but the level of details taken into account is higher. This level of detail increases in the following dimensions: (i) the time is measured in a smaller unit, e.g. days or hours; the process may be continuous, (ii) the product demand is defined more precisely, and (iii) the facility is not considered as a single entity. In fact, each facility is a collection of resources or machines. Each product has to undergo a number of operations on different machines. Each product has a specific route and given processing requirements on different machines. The demand for each individual product within a family is taken into account. The key parameters at this level are the individual due dates of the orders, sequence-dependent setup times, sequence-dependent setup costs, lead times, and the costs of the resources (Kreipl & Pinedo, 2004).

In his comprehensive review, Kallrath (2002a) categorizes the scheduling problems into (1) batch and campaign planning, (2) scheduling problems in the chemical process industry including lot-sizing and sequencing, (3) time-precedence and aggregate resource constraints, and (4) nonlinear scheduling problems including blending. Body of literature in this category is tremendous. Earliest works in this field go back to the late 70s (Takamatsu, Hashimoto, & Hasebe, 1979), (Mauderli & Rippin, 1979), with a major focus on the scheduling of batch systems. In 80s and 90s, it gets more attention (Janicke, 1984), (Egli & Rippin, 1986) and incorporating scheduling issues in the design problems is started (Birewar & Grossmann, 1989). Bassett, Pekny, and Reklaitis (1997) apply scheduling concepts to identify more realistic operating policies for a batch processing facility. Cerda, Henning, and Grossmann (1997) address the short-term scheduling of single-stage multiproduct batch plants with parallel lines. Mendez, Henning, and Cerda (2000) work on scheduling of batch plants taking into account different order due dates. Mendez and Cerda study the dynamic scheduling of multi-product batch plants (2003) and propose a mixed integer linear programming (MILP) framework for scheduling batch processes with limited discrete resources (2004).

As a result of high complexity of scheduling models, most of the works in this context have been done on the mathematical aspects of the problem. Lots of articles can be found which introduce models that try to solve complex problems in a very short time. Mendez, Cerda, Grossmann, Harjunkoski, and Fahl (2006) give a broad review of optimization techniques used in scheduling problems. Moreover, due to the strong link between planning and scheduling activities, some researchers worked on the integration of these two levels (Burkard, Hujter, Klinz, Rudolf, & Wennink 1998), (Rodrigues, Latre, & Rodrigues, 2000), (Zhu & Majozi, 2001) and (Erdirik Dogan & Grossmann, 2006).

1.1.2 Supply chain modeling

An SC problem, no matter it is a design, a tactical or an operational problem, is formulated into an optimization problem and is solved to maximize the profit or minimize the costs and risks. In an optimization problem, the first step is to formulate the problem into a mathematical model, i.e. a set of mathematical relationships (e.g. equalities, inequalities, logical conditions) which demonstrate an abstraction of the real world problem. The mathematical model can be static (steady-state), dynamic (multi-period), deterministic or stochastic (Papageorgiou, 2009). A mathematical model in an optimization problem comprises four key objects (Kallrath, 2000):

- Data or parameters, which typically include the constants of the model
- Decision variables, including continuous, semi-continuous, binary integer
- Constraints, including equalities and inequalities
- Objective function

Mathematical models for optimization usually result in structured problems such as (Kallrath, 2000):

- Linear programming (LP) problems
- Mixed integer linear programming (MILP) problems
- Nonlinear programming (NLP) problems
- Mixed integer nonlinear programming (MINLP) problems

There are two types of decision variables in optimization problems. The first type is those which are treated as continuous variables, representing continuous degrees of freedom, e.g., the amount of a product which must be produced in a manufacturing site. On the other hand, integer variables are involved in mixed integer, combinatorial or discrete optimization problems. Such variables are restricted to, for example, counts (number of production-distribution sites), decisions (yes/no), or logical relations (if product A is produced then product B also needs to be produced) (Kallrath, 2000). Depending on the level of the SC, i.e. strategic, tactical or operational, the SC decision variables involve (Papageorgiou, 2009):

- Number, size and location of manufacturing sites, warehouses and distribution centres, and the resources inside them
- Production decisions related to plant production planning and scheduling

- Network connectivity (e.g. allocation of suppliers to plants, warehouses to markets etc.)
- Management of inventory levels and replenishment policies
- Transportation decisions concerning mode of transportation (e.g. road, rail etc.) and also sizes of material shipments

SC optimization problems are often categorized as mixed integer optimization problems, because they may involve integer variables, and can be in the form of linear or nonlinear mixed integer problems. Most of the real world problems in process industries face with different types of mixed integer optimization. Kallrath (2000) provided a list of problems in this context;

- Production planning (production, logistics, marketing) - MILP, MINLP
- Sequencing problems (putting production into order) – MILP
- Scheduling problems (production of goods requiring machines and/or other resources)
- Allocation problems (e.g., allocating resources to orders, people to tasks)
- Distribution and logistics problems (supply chain optimization) – MILP
- Blending problems (production and logistics) - LP, MILP, NLP, MINLP
- Refinery planning and scheduling (refineries, chemical process industry) - NLP, MINLP
- Process design (chemical process industry, food industry, refineries) – MINLP
- Engineering design (all areas of engineering) - NLP, MINLP
- Selection and warehouse/depot location problems (strategic planning) – MILP
- Investment and de-investment design problem (strategic planning) – MILP
- Network design (planning, strategic planning) - MILP, MINLP
- Financial problems (strategic planning) - MILP, MINLP

1.1.3 Uncertainty in supply chain analysis

One of the key issues in SC problems, either design or tactical/operational, is the uncertainties existing at different nodes of the supply chain network. Uncertainties arise from suppliers, manufacturers and customers (Davis, 1993). More specifically, uncertainty exists in product demand and prices, raw material availability, product launch, geopolitical changes (Papageorgiou, 2009). Suppliers can be characterized through their past performance and their responsiveness. Manufacturing and production issues can be addressed using reliability and maintenance analysis for the equipment. Finally, customer demands must be addressed through high quality forecasting methods. From a generic point of view, the sources of uncertainty can be identified as lack of information, complexity of information, conflicting evidence, ambiguity, and measurement errors (Zimmermann, 2000).

Most researches on addressing uncertainty can be categorized into two primary approaches; probabilistic approach and the scenario planning approach (Tsiakis, Shah, & Pantelides, 2001), though the choice of the pertinent approach depends on the problem context, because there is no single theory being capable of modeling all kinds of uncertainty (Zimmermann, 2000). Probabilistic models capture the uncertainty aspects of the supply chain treating one or more parameters as random variables with known probability distributions, while scenario planning tries to contemplate uncertainty by representing it in terms of a moderate number of discrete realizations of the stochastic quantities, constituting distinct scenarios. Complete realization of all uncertain parameters results in a scenario. The objective is to find solutions which perform well under all scenarios (Tsiakis, Shah, & Pantelides, 2001).

An extensive classification and study has been done by Sahinidis (2004), who addressed the main approaches to optimization under uncertainty. He categorized them as (1) stochastic programming including recourse models (stochastic linear programming, stochastic integer programming, stochastic non-linear programming, robust stochastic programming), and probabilistic models, (2) fuzzy programming (flexible and possibilistic programming), and (3) stochastic dynamic programming. Other comprehensive reviews on optimization under uncertainty can be found in Cheng, Subrahmanian, and Westerberg (2005) and Li and Ierapetritou (2008).

Optimization under uncertainty began in 50s and evolved quickly in both theory and algorithm (Sahinidis, 2004). Over the last decades, SC optimization under uncertainty is studied widely. Liu and Sahinidis (1996) develop a multi-scenario multi-period optimization model, using projection techniques for improving the efficiency of solution process, to address the uncertainty in demand and price. Iyer and Grossmann (1998) introduce a model which determines the optimal selection and expansion of processes over a long-range planning horizon, incorporating uncertainty in terms of demands and prices of chemicals, by utilizing multiple scenarios for varying situation. BiLevel decomposition is applied to enhance the computation of this model. Applequist, Pekny, and Reklaitis (2000) study risk management in chemical SC investments.

They introduce the risk premium approach to determine the right balance between expected value of investment performance and associated variance. An investment decision is approved, when its expected return is better than the corresponding ones in the financial market with similar variance. Gupta, Maranas, and McDonald (2000) employed twp-stage stochastic programming to address mid-term SC planning under demand uncertainty. In order to resolve the challenge associated with obtaining the second stage recourse function, firstly a closed-form solution of the inner optimization problem is obtained, using linear programming duality, followed by expectation evaluation by analytical integration. In addition, analytical expressions for the mean and standard deviation of the inventory are derived and used for setting the appropriate customer demand satisfaction levels in the supply chain. Tsiakis, Shah, and Pantelides (2001) introduce demand uncertainty by using a scenario-based approach with each scenario representing a possible future outcome and having a given probability of occurrence. Barbaro and Bagajewicz (2004) present a methodology which addresses financial risk management using two-stage stochastic programming for planning under uncertainty. A known probabilistic definition of financial risk is adapted to be used in the framework of two-stage stochastic programming and its relation to downside risk is analyzed. Romero et al. addressed the integration of budgeting models into planning and scheduling models for the chemical batch industry, using a two-stage model in which at first the scheduling and planning problem of the batch specialty chemical plant is optimized in order to fulfill the due date policy. At the next stage, a deterministic cash management model is optimized to maximize the enterprise earnings, using the cash flows of the scheduling-planning model as parameters. Guillen, Mele, Bagajewicz, Espuna, and Puigjaner (2005) address problem of uncertainty when SC design and tactical/operational level activities are integrated.

In summary, as stated by Papageorgiou (2009), SC optimization under uncertainty is a field of growing interest and thus, methodologies are still emerging. However, there are some issues remaining to be addressed in this including (1) accurate characterisation of uncertainty and (2) the numerical solution of the large-scale problems that inevitably arise in this context.

1.1.4 Forest biorefinery supply chain

Figure 1-1 illustrates the SC of an FBR. The final goal of the SC of an FBR is to recover more of the biomass left in the forest, to generate energy, to produce fuels and to extract chemicals from wood. Several types of feedstock, ranging from forest biomass to recycled papers and agricultural residues, can be used. Feedstock is transported to the mills, then treated and prepared to be processed. The final products involve wood and paper products, biofuel, green chemicals and energy.

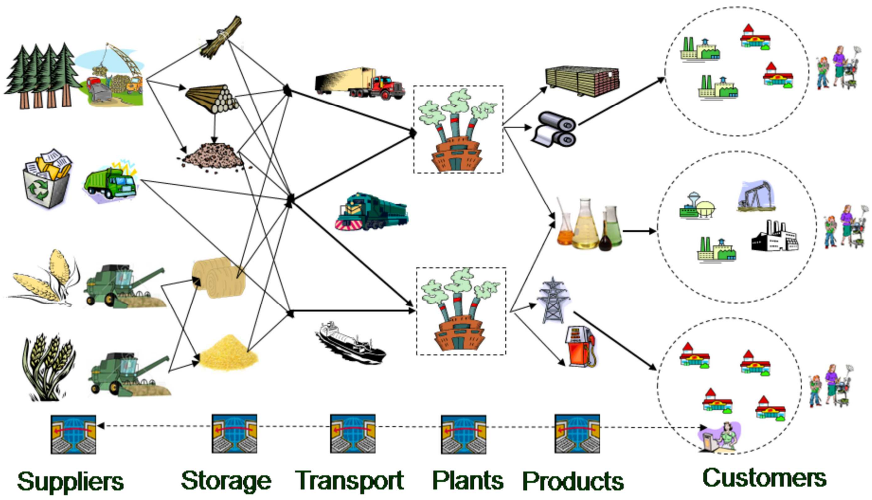


Figure 1-1 Forest biorefinery supply chain

The biorefinery technologies which are currently under development, are typically classified into biochemical processes and thermochemical processes. The biochemical processes are based on chemical fractionation and metabolic transformation of forest biomass, while the thermochemical processes are based on gasification/pyrolysis of carbon based byproducts and residues in pulp mills (Wising & Stuart, 2006). Wising and Stuart (2006) showed that hemicellulose extraction and lignin precipitation as biochemical pathways, and black liquor gasification/pyrolysis as a thermochemical pathway have the potential to be integrated with P&P processes. According to the characteristics of these pathways, each of them can be employed via a specific implementation strategy. Hytonen (2011) divide the biorefineries into adjacent biorefineries and tightly integrated biorefineries. Adjacent processes use the existing assets, but do not interfere with the pulp and papermaking material balances. Examples are production of pellets or transportation biofuels from forest or agricultural based feedstocks. On the contracy, tightly integrated biorefinery processes are also exchanging material with the P&P processes. Hemicelluloses extraction from wood chips prior-to-pulping, lignin separation from black liquor, or black liquor gasification for chemical recovery, and energy and bio-product production are major instances of processes that can be used in integrated biorefineries. As mentioned earlier, an implementation strategy can be coupled with a specific process in a pathway. Below are the processes that can be suitable for an integrated biorefinery strategy:

- Green liquor extraction of hemicelluloses for ethanol and biochemicals production
- Hot-water hemicellulose extraction to produce biofuels and biochemicals
- Partial dilute-acid pre-hydrolysis of loblolly pine for hemicellulose extraction prior-to-cooking for ethanol production
- Black liquor gasification combined cycle system for Tomlinson recovery boiler replacement and simultaneously biofuels production
- Carbon dioxide and sulphuric acid utilization for lignin precipitation and filtration from black liquor

Adjacent strategies can accommodate the following processes:

- Steam-reforming or
- Gasification of bark and forest biomass followed by Fischer-Tropsch liquids synthesis
- First-generation biofuels production

Biorefinery is a new area of study and research related to the biorefinery SC just started in the last decade. In one of the first attempts, Tembo, Epplin, and Huhnke (2003) introduce an MILP model for a multi-region, multi-period problem in lignocellulosic biomass-to-ethanol industry, comprising of alternative feedstocks, feedstock production, delivery, and processing. The objective of this work is to determine, for specific regions in Oklahoma, the most economical source of lignocellulosic biomass, timing of harvest and storage, inventory management, biorefinery size, and biorefinery location, as well as the breakeven price of ethanol, for a gasification-fermentation process. Sammons, Eden, Yuan, Cullinan, and Aksoy (2007) propose a general systematic framework including fixed and variables production cost calculation, pinch analysis, and SC optimization for optimizing product portfolio and process configuration in integrated biorefineries. The framework generates data for economic and environmental performance metrics. Tursun, Kang, Onal, Ouyang, and Scheffran (2008) develop a mathematical programming model that determines optimal locations and capacities of biorefineries, delivery of bioenergy crops to biorefineries, and processing and distribution of ethanol and co-products across Illinois. Slade, Bauen, and Shah (2009) analyze the role of SC design on determining the viability of commercial cellulosic ethanol projects in Europe.

Eksioglu, Acharya, Leightley, and Arora (2009) introduce a mathematical model to design a biomass-to-biorefinery SC, and to analyze and manage its logistics through the coordination of long-term and short-term decisions. Given the availability of biomass feedstock, as well as biomass transportation, inventory and processing costs, the model determines the number, size and location of biorefineries needed to produce biofuel and the amount of biomass shipped, processed and inventoried during a time period. Mansoornejad, Chambost, and Stuart (2010) develop a systematic hierarchical methodology to integrate product portfolio design with SC network design in the FBR. Separate methodologies for product portfolio definition, process technology selection, and SC design are integrated in the proposed hierarchical methodology. It is described how these methodologies along with other analysis tools such as LCA can provide metrics and criteria to be used in a multi-criteria decision-making (MCDM) framework for making the final decision. Sharma, Sarker, and Romagnoli (2011) introduce a model for assessing the impact of feedstock and technology selection, process and utility integration, and effluent recycle for a multi-product multi-platform biorefining enterprise. Kim, Realff, and Lee (2011) present a model for the optimal design of biomass SC networks under uncertainty, covering an SC located in the Southeastern region of the United States. The SC consists of biomass supply locations and amounts, candidate sites and capacities for two kinds of fuel conversion processing, and the logistics of transportation from the locations of forestry resources to the conversion sites and then to the final markets. A two-stage stochastic approach is used to solve the MILP with the objective of maximizing the expected profit over different scenarios. The robustness and global sensitivity analysis of the nominal design (for a single nominal scenario) vs. the robust design (for multiple scenarios) are analyzed using Monte Carlo simulation. Giarola, Zamboni, and Bezzo (2011) present an MILP framework for the strategic design and planning of corn grain and stover-based bioethanol SCs through first and second generation technologies, which optimizes the environmental and financial performances simultaneously. Bowling, Ponce-Ortega, and El-Halwagi (2011) introduce a systematic approach for the optimal production planning and facility placement of a biorefinery using an optimization formulation which specifically determines the optimal SC, size, operational strategies, location of the biorefinery and pre-processing hub facilities, and selection of biomass to maximize overall net profit. The model takes into account non-linear economy-of-scale behavior of the capital cost functions that are reformulated using disjunctive models to yield convex relationships to guarantee a global optimal solution. Marvin, Schmidt, Benjaafar, Tiffany, and Daoutidis (2012) study the NPV of a biomass-to-ethanol SC in a 9-state region in the Midwestern United States, using an MILP to find optimal locations and capacities of biorefineries in conjunction with biomass harvest and distribution. Monte Carlo simulation is performed to investigate the robustness of the SC and whether or not the proposed biorefineries will be built or will fail financially after being built. Table 1-1 summarizes the key issues addressed by the biorefinery SC literature.

Table 1-1 Biorefinery SC literature

	Strategic decision making	**SC network design**	**SC management**
Tembo et al. (2003)	Source of biomass Timing of harvest and storage Biorefinery size	Biorefinery location	Inventory management
Sammons et al. (2007)	Product portfolio Process configuration		
Tursun et al. (2008)	Biorefinery size	Biorefinery location	Feedstock delivery Product delivery Process planning
Slade et al. (2009)	Viability of commercial cellulosic ethanol projects in Europe		
Eksioglu et al. (2009)	Biorefinery size	Biorefinery location	Biomass shipped, processed & stored
Mansoornejad et al. (2010)	Product portfolio Process technologies & capacity	Capacity of SC nodes Partnership	
Sharma et al. (2011)	Feedstock & technology selection Process & utility integration		
Kim et al. (2011)	Biorefinery capacities	Biomass supply locations & amounts Biorefinery location	Logistics of transportation
Bowling et al. (2011)	Biorefinery capacity Selection of biomass	Biorefinery location Location of pre-processing hubs	Production planning Operational strategies
Marvin et al. (2012)	Biorefinery capacity	Biorefinery location	Biomass harvest and distribution

Feedstock procurement and biomass supply is a big challenge for biorefinery (Reynolds, 2002). Thus far, research on biomass SC has provided models that estimate the cost of collecting, handling and hauling biomass to biorefineries, compare different modes of delivering biomass, and identify SC options for bio-based businesses (Eksioglu, Acharya, Leightley, & Arora 2009).

1.2 Margins-based operating policy

In 2004, Shapiro stated in one of his articles that "Current supply chain network optimization studies are still too timid and limited". He believed that, in too many companies, purchasing, manufacturing and distribution planning activities are not well integrated. Moreover, even when all SC sections are taken into consideration, the objective is often minimizing the total SC cost associated with fixed and given demand over a future planning horizon, while the objective could have been maximizing net revenues by letting sales vary. In other words, the firm does not exploit the potential of coordinating supply chain and demand management decisions to maximize net revenue. The demand management decisions depend on the nature of the company's industry. For commodity industries with price-driven sales such as forest products or petrochemicals, the SC network optimization model could consider revenue functions derived from product price elasticities in order to optimize the production of its product (Shapiro, 2004). What can be observed in the literature is that some industries have recognized the importance of profit maximization compared to cost minimization, while some other industries still miss this vision.

One of the objectives of this thesis is to compare these two approaches, i.e. one based on profit maximization and one based on cost minimization, for the case of FBR. In the following sections both approaches are defined and some examples are given for each of them.

1.2.1 Margins-based approach in process industries

Based on Shapiro's discussion, an appropriate and ambitious approach in SC management would have three dimensions; first, the SC must be seen as a whole and all SC nodes must be considered in the analysis. Second, the objective function must be profit maximization, instead of cost minimization. Lastly, the potentials of an SC for being flexible to be adapted to market conditions must be exploited. A margins-based approach takes this strategic view and aims at (1) maximizing profit (2) over its SC (3) by exploiting the flexibility that is inherent in the SC.

Technically, margin or profit margin is defined as a ratio of profitability calculated as net income divided by revenues, or net profits divided by sales. In the margins-based approach, margin simply refers to profit. The objective function in a margins-based SC model is the profit to be maximized. The margins-based SC model considers all SC sections and is allowed to exploit the inherent flexibility of these sections, i.e. flexibility of feedstock types and feedstock resources, process flexibility including product flexibility and volume flexibility (which are discussed in details in the next section of literature review), flexibility in inventory level, flexibility in delivery, etc. Using SC flexibility, the margins-based policy maximize the profit by choosing the right orders at the right time, considering product price in the market, and producing the right product in the right amount. This approach might increase the likelihood of changeovers and varying production rates, which in turn increases the production cost. But, these changes are justifiable, as long as they improve the profit in a way that it compensates the rise in the production cost.

Vidal and Goetschalckx (1997) and Beamon (1998) present comprehensive studies on the SC optimization problems and performance measures used in them, being addressed in the studies carried out in 90s. The most popular performance measure used as the objective function was the cost and there were few studies which used profit as the objective function. A decade later, Verderame, Elia, Li, and Floudas (2010) categorizes the objective functions used in SC optimization models developed for chemical, petrochemical and pharmaceutical industries into profit maximization within a finite time horizon, the minimization of costs associated with production and/or customer dissatisfaction within a finite time horizon, and makespan minimization. In recent years, there has been a shift toward considering profit as the objective function along with minimizing risks, losses or environmental and/or social impacts (Papageorgiou, 2009), (Verderame, Elia, Li, & Floudas 2010), though, as stated by Pinto-Varela, Barbosa-Póvoa, and Novais (2011), “the majority of cited papers feature a cost minimization objective, also noticing that very few articles refer to models subject to multiple and conflicting objectives covering both profit and environmental aspects”.

Pharmaceutical industry has very well applied profit/NPV maximization in its SC models. As mentioned by Shah (2004), “Most strategic/infrastructural decisions have historically been based on NPV or some form of expected NPV, which in turn utilise weighted average costs of capital or some required return on investment”. Example of this can be found in (Papageorgiou, Rotstein, & Shah, 2001; Gatica, Papageorgiou, & Shah, 2003; Levis & Papageorgiou, 2004; Shah, 2004; Sousa, Shah, & Papageorgiou, 2005; Sousa, Shah, & Papageorgiou, 2008). Same approach can be seen in refinery and petrochemical SC optimization problems. The objective function is mainly profit in these cases. Examples can be viewed in (Pinto, Joly, & Moro, 2000), (Neiro and Pinto, 2004), (Pitty, Li, Adhitya, Srinivasan, & Karimi, 2008), (Kim, Yun, Park, Park, & Fan, 2008) and (Khor, Elkamel, Ponnambalam, & Douglas 2008).

1.2.2 Manufacturing-centric approach in pulp and paper industry

For years, P&P industry lagged other industries in terms of investment and development in SC projects. At the present time, this lack of investment is going to decrease by large expenditures recently made by many P&P companies, especially in IT. One of the most influential reasons for this new approach is the awareness that P&P industry is behind others, as well as the hope for bringing the long sought-after level of business returns by means of SC operations improvements (Lail, 2004). An extensive survey was done during July – October 2005 regarding the status of P&P industry concerning SC management and 11 European paper companies participated in the survey. The results revealed that, besides being a major cost and working capital factor, SC management can also be considered as a source of significant competitive edge (Uronen, 2006).

The operating policy in the P&P industry is said to be “manufacturing-centric.” Lail (2003) identifies the distinctions between P&P industry and other process industries, which ultimately lead to such an approach for the operating policy. A major difference between P&P SC and other process industries’ SC is the organizational distinction between scheduling and purchasing functions. In other words, different sections of the P&P SC are considered separately. Another difference stems from the fact that P&P industry is unusually capital-intensive. Therefore, the industry participants always try to use the machine capacity efficiently and effectively. As a result, capacity management is primary, while the material management is secondary (Lail, 2003), and process efficiency is viewed as the key measure for profitability, and thus it is believed that minimizing production cost will result in the highest profitability (Dansereau, El-Halwagi, & Stuart 2009). By treating the manufacturing process as the focal point, inventory and changeover costs are typically ignored or considered separately (Lail, 2003), and SC costs are often neglected, resulting in lower profitability (Dansereau, El-Halwagi, & Stuart 2009). Moreover, in order to minimize the cost, production planning assumes a known set of orders and a fixed sequence of product grades and the capability of the process for flexibility in manufacturing and changeover is not used. This can result in decreasing the profitability of the company when prices or demands change. Suppose that, based on the pre-defined production sequence, the company has produced some products that in a particular period, are subject to low price or weak demand (unlike lumber industry, another sector in forest industry, whose market is always strong). In case of low price, it is obvious that profit declines. In case of weak demand, the company should store its products for a longer period, in which case the inventory cost rises. In such a case, the company might sell its products at a discount, which would decrease the profit. Moreover, some companies take orders based on their sequences, and they miss out on better orders just because these orders do not fit their production sequence.

As mentioned earlier, one of the key aspects of manufacturing-centric policy is its cost-minimization approach. This approach can be seen in the P&P SC optimization researches. Bredstrom, Lundgren, Ronnqvist, Carlsson, and Mason (2003) study the SC problem of a large international pulp producer with five pulp mills located in Scandinavia which uses manual planning for most of its SC, including harvesting and transportation of pulp, production scheduling and distribution of products to customers. They developed MILP models that determine daily SC decisions over a planning horizon of three months. The objective function is the total cost to be minimized. Karlsson, Rönnqvist, and Bergström (2004) address annual harvesting planning from the perspective of Swedish forest companies. The objective function is the total cost to be minimized, including harvesting cost, road-opening cost, cost of purchased logs, transportation cost, storage cost, and different penalties. Carlsson and Ronnqvist (2005) present a procurement model for a pulp mill in Sweden, which focuses on minimizing the cost associated with direct and backhaulage transport as well as sorting cost. Bouchriha, Ouhimmou, and D'Amours (2007) introduce a mathematical model for lot sizing problem on paper machines, where a predetermined production sequence must be maintained. The objective is to minimize the total inventory, setup and production costs for all products over the entire planning period. Jones and Ohlmann (2008) study a vertically integrated papermaking operation composed of an integrated pulp and paper mill with its regional supply network. They develop a model for long-range planning of timber supply. The objective is to minimize cost of bare land, cost of procuring the timber content of a normal forest with a t-year harvest rotation, and the discounted cost of managing the normal forest for wood chip and lumber production over an infinite horizon.

However, there are a few studies which apply a profit-oriented approach. An example can be seen in Beaudoin, LeBel, and Frayret (2007).

1.2.3 Critical analysis

Margins-based policy, which is a profit-oriented approach, is getting attention in different chemical process industries and its value is now obvious to some industrial sectors. However, in forestry and P&P industry it is not still a part of manufacturing culture. As biorefinery is going to be implemented by forestry and P&P companies, it is critical to prove that, given other industrial sectors' experiences, a margins-based approach can add value and thus, can be applied in future biorefineries. Therefore, it is of crucial importance to analyze the performance of the manufacturing-centric approach and the margins-based approach in today's volatile market, and to compare their consequences. The design of a plant is directly related to its operating policy. Hence, when the operating policy of a future industry is defined, it can be designed based on the defined operating policy. Margins-based operating policy focuses on exploiting flexibility throughout the SC. Therefore, identifying whether or not the margins-based policy is an appropriate option for future biorefineries affects the design activities.

1.3 Metrics for supply chain design and analysis

An important issue in the design and analysis of an SC is developing relevant performance measures or metrics. Such metrics can be used for two major purposes; they can be used in designing systems by determining the values of the decision variables that yield the most desirable level(s) of performance. Moreover, they can be applied to determine the efficiency and effectiveness of an existing system, and thus to compare the performance of competing alternative systems (Beamon, 1998).

Beamon (1998) provides an inclusive summary of performance metrics and categorizes them into two classes; qualitative and quantitative. Qualitative measures imply no single direct numerical measurement, though some aspects of them may be quantified. Such measures include: customer satisfaction, flexibility, information and material flow integration, effective risk management, and supplier performance. On the other hand, quantitative measures are directly described numerically. They can be classified into two categories; measures whose objectives is based on cost or profit, and measures whose objective is somehow related to a measure of customer responsiveness. In this regard, measures based on cost/profit include cost minimisation, sales maximisation, profit maximisation, inventory investment minimisation and return on investment. Measures based on customer responsiveness consist of fill rate maximisation, product lateness minimisation, customer response time minimisation, and lead time minimisation. These measures can be used as the objective function in the mathematical formulations.

An important issue to be considered for a system in a volatile environment is the robustness of that system against volatility. Klibi, Martel, and Guitouni (2010) define robustness of an SC network as the extent to which the network is able to carry its functions for a variety of plausible future scenarios. The concept of robust design in chemical engineering is an area of interest (Georgiadis & Pistikopoulos, 1999; Bernardo, Pistikopoulos, & Saraiva, 1999; Bernardo, Pistikopoulos, & Saraiva, 2001). In the area of SC design and planning, the concept of robustness has been addressed in two different ways; some studies focus on the issue of robust optimization, in which a few number of parameters and constraints are added to the mathematical formulation to limit the variables and the objective function for making the solution more robust. An example can be seen in (Verderame & Floudas, 2011). Some other studies use metrics for quantifying robustness of SC planning. Several robustness metrics have been introduced by Vin & Ierapetritou (2001) for improving the scheduling of multi-product batch plants under demand uncertainty.

Another issue that can be addressed in volatile and uncertain environment regarding the performance of a system is flexibility. Flexibility is discussed in the next part of the literature review. Quantifying flexibility has been another issue that gained attention. Beamon (1998) gives a generic definition of a flexibility measure for SC: The degree to which the supply chain can respond to random fluctuations in the demand pattern. In systems engineering, many works are done on the issue of flexibility based on the work of Swaney and Grossmann (1985). They define flexibility index as a metric that characterizes the size of the region of feasible operation in the uncertain parameter space. Another measure of flexibility is introduced by Voudouris (1996) which defines flexibility as the ability of the system to absorb unexpected demand.

1.3.1 Critical analysis

The classic robustness metrics somehow give an average representation of the system's performance against volatility, i.e. they calculate an average deviation of a variable in several scenarios from the desirable value of that variable. This approach cannot consider the number of scenarios, and thus, makes it difficult for interpretation. Therefore, there is a need for a metric that can consider the number of scenarios, especially those which have a worse performance compared to the average or base-case scenario. Moreover, the flexibility index is defined based on the uncertain parameter. Having a metric that, instead of being related to uncertain parameter, is linked to the flexibility of processes itself can be very helpful in analyzing and designing the flexibility of processes.

1.4 Manufacturing flexibility

In this section, different definitions of flexibility and the problems studied to date related to flexibility are presented. Next, different types of flexibility are introduced and finally, a concrete definition is provided of the concept of flexibility which forms the basis of the methodology presented in this thesis.

1.4.1 Definition

One of the earliest definitions of flexibility goes back to Ropohl (1967), who introduces flexibility as "the property of the system elements that are integrally designed and linked to each other in order to allow the adaptation of production equipments to various production tasks". Another early definition of flexibility was proposed by Gupta and Goyal (1989), who define it as "the ability of a manufacturing system to cope with changing circumstances or instability caused by the environment". From an operational point of view, Nagarur (1992) defines flexibility as "the ability of the system to quickly adjust to any change in relevant factors like product, process, loads and machine failure". Upton (1994) provides a broader definition which addressed flexibility as "the ability to change or react with little penalty in time, effort, cost or performance". Sethi and Sethi (1990) did a comprehensive survey on this concept, reviewing different definitions and types of manufacturing flexibility. They define the flexibility of a system as its adaptability to a wide range of possible environments that it may encounter. In other words, a flexible system must be capable of changing to deal with a changing environment.

In the chemical engineering context, Grossmann, Halemane, and Swaney (1983) define flexibility as the ability of a manufacturing system to satisfy specifications and constraints despite variations that may occur in parameter values during operation.

From a hierarchical decision-making point of view, flexibility can be classified as long-term (strategic), midterm (tactical), and short-term (operational) flexibility. These levels can be defined respectively as: (i) the ability of a system to respond to changes in strategy, new product introductions, and basic design changes, (ii) the ability to operate at varying rates, to accept random, minor changes, and to convert the plant for alternative uses, and (iii) the ability to reset and readjust between known production tasks to permit a high degree of variation in sequencing and scheduling (Beach, Muhlemann, Price, Paterson, & Sharp 2000).

Several reasons have been mentioned for the importance of flexibility. Frazelle (1986) believes that flexibility is required to maintain competitiveness in a changing business environment of which the critical features are rapidly-decreasing product half-life, the influx of competitors, an increasing demand for product changes, and the introduction of new products, materials, and processes. Slack (1983) sees the incentives for flexibility in the instability and unpredictability of the manufacturers' operational environment and in developments in production technology.

1.4.2 Flexibility problems

Flexibility problems can be classified into two groups: flexibility design and flexibility analysis.

1.4.2.1 Flexibility design

In this type of problem, the design is unknown and the objective is to find the optimal design of a system considering the costs incurred by that design. A design representing a higher degree of flexibility will have a lower probability of facing infeasible operating conditions, but at a higher cost. Two major areas have been considered by Grossmann, Halemane, and Swaney (1983): optimal design with a fixed degree of flexibility, and design with an optimal degree of flexibility.

1.4.2.1.1 Optimal design with a fixed degree of flexibility

The flexibility of a design is optimal when the economic advantages of flexibility are balanced in relation to its cost. In this type of problem, a design should be identified that can operate over varying conditions. These varying conditions must be specified as a bounded range of parameter values over which the design is able to meet the specifications at minimum cost. In this type of problems the required degree of flexibility has already been specified, either by a discrete set of required operating conditions, or by requiring feasibility of operation when a set of uncertain parameters varies between fixed bounds. Therefore, this class of problem can be divided into two categories (Grossmann, Halemane, & Swaney 1983):

a) Deterministic problems or problems of deterministic multiperiod design, in which the plant is designed to operate optimally under various conditions over a sequence of time periods. The goal is to ensure that the plant will be able to meet the specifications over successive periods of operation.

b) Stochastic problems or problems of design under uncertainty, which address the design of chemical plants under conditions where the values of some of the process parameters have significant uncertainty. However, a particular design problem as presented might include both these problems.

The ultimate goal in solving these types of problems is to ensure that the design, while being economic, meets the specifications under different imposed conditions.

1.4.2.1.2 Design with optimal degree of flexibility

In this type of problem, the desired degree of flexibility is not known, and a design with the optimal degree of flexibility must be identified. The optimal degree of flexibility does not necessarily imply the highest degree of flexibility, because another criterion, which is the cost of the design, is important in determining optimality of a design. In fact, design with optimal degree of flexibility addresses problems which needs establishing a trade-off between the cost of the plant and its flexibility. Therefore, the objective function can be separated into two components: minimizing capital and operating costs on one hand, and maximizing flexibility on the other hand. The result will be a trade-off curve which relates flexibility and cost.

The major task in this type of problem is to determine the degree of flexibility. In other words, a metric or a quantitative measure of flexibility in the form of a scalar index is needed that can measure the size of the region of feasible operation for the design. This metric is called the *flexibility index*. The value of flexibility index characterizes the size of the region of feasible operation in the uncertain parameter space. In other words, it can be defined as the largest-scale deviation of any of the expected deviations that the design can handle and still operate feasibly (Swaney & Grossmann, 1985). Flexibility-index problems involve designing the plant with the aim of both cost minimization and flexibility-measure maximization. Problems in this category have evolved from flexibility-index problems (Swaney & Grossmann, 1985) to stochastic flexibility-index problems (Pistikopoulos & Grossmann, 1988) and expected stochastic flexibility-index problems (Straub & Grossmann, 1988).

1.4.2.2 Flexibility analysis

In flexibility analysis problems, the design of the plant is given, and the goal is to analyze the plant's capability for feasible operation. Two types of problems can be defined in this category;

1.4.2.2.1 Feasibility or flexibility test

In this type of problem, it is determined whether the design can operate feasibly at all uncertain points in the range. More specifically, the objective of the feasibility problem is to determine whether, for a given design, a set of nominal values for the uncertain parameters, a set of expected deviations in the positive and negative directions, and a set of constraints, at least one set of control variables can be chosen during plant operation such that, for every possible realization of the uncertain parameters, all the constraints are satisfied (Bansal, Perkins, & Pistikopoulos, 2002). Halemane and Grossmann (1983) carried out one of the earliest studies in this domain and showed how, for a given design and a fixed parameter value, the max-min-max problem provides a measure of the size of the feasible operating region. Grossmann and Floudas (1987) presented mathematical formulations for the feasibility test based on the property that the number of active or limiting constraints on flexibility is equal to the number of control variables plus one, provided there is linear independence among the active constraints. Bansal, Perkins, and Pistikopoulos (2000) introduced a unified theory and algorithms based on multi-parametric programming techniques for the solution of feasibility test problems in linear process systems. Floudas, Gumus, and Ierapetritou (2001) presented an approach for feasibility test problems based on the principles of the αBB deterministic global optimization algorithm, which relies on a difference-of-convex-functions transformation and a branch-and-bound framework. Goyal and Ierapetritou (2003) developed an algorithm for evaluating the feasibility of non-convex processes, based on the idea of systematically determining the infeasible areas using an outer approximation procedure and a simplex approximation approach to approximate the expanded feasible space which can be constructed by the exclusion of non-convex constraints.

1.4.2.2.2 Flexibility index

The aim of flexibility-index problems is to determine how flexible a given design is. In other words, the maximum deviation that the design parameters can tolerate is determined. Again, the major issue in these problems is to define a quantitative measure for the degree of flexibility. Index of flexibility or *flexibility index* can be used for this class of problems.

Grossmann and Floudas (1987) addressed the analysis of the flexibility of a proposed design using an active constraint strategy and MINLP formulations for flexibility-index problems. Pistikopoulos and Grossmann (1988) worked on redesigning existing process flowsheets to increase their flexibility. The major difficulty in such retrofit problems is that of deciding which parameter or structural changes are required, with the aim of increasing flexibility at the least investment cost. Their proposed approach for the retrofit design problem involves: (a) a systematic procedure for handling parametric changes of the design variables, (b) embedding a strategy for handling simultaneous structural and parametric changes, and (c) a procedure for developing tradeoff curves between cost and flexibility. Bansal, Perkins, and Pistikopoulos (2000) presented algorithms based on multi-parametric programming techniques for the solution of flexibility analysis and design optimization problems in linear process systems which are used to solve flexibility-index problems in systems with deterministic parameters. The algorithms as developed are computationally efficient and reveal explicitly the dependence of various flexibility metrics on the values of the continuous design variables.

1.4.3 Flexibility types

Many efforts have been made to categorize various types of flexibility. The common element in all types of flexibility is that flexibility is used to mitigate the risks associated with different types of uncertainty. These uncertainties are the results of variations in the temperature, pressure, or flowrate of a stream, changes in the state of equipment, or fluctuations in the price and demand of products. Based on the type of uncertainty, specific types of flexibility can be defined. Sethi and Sethi (1990) introduce 50 different terms for different types of flexibility, although their definitions were not always precise and, for identical terms, not always in agreement with one another. Swamidass (1988) points out the difficulties of understanding and therefore categorizing flexibility to be (i) the use of flexibility terms with overlapping scopes, (ii) the use of flexibility terms with different meanings and (iii) the use of flexibility terms which are aggregates of others. Beach, Muhlemann, Price, Paterson, and Sharp (2000) carry out a comprehensive survey on the concept and types of flexibility and concluded that the original eight categories of flexibility defined by Browne, Dubois, Rathmill, Sethi, and Stecke (1984) represent the most comprehensive classification of flexibility. They classified manufacturing flexibility in discrete manufacturing environments into eight categories: machine, process, product, routing, volume, expansion, operation, and production.

In the chemical engineering context, four major types of flexibility have been widely studied: recipe (Verwater-Lukszo, 1998; Romero, Espuna, Friedler, & Puigjaner 2003; Ferrer-Nadal, Puigjaner, & Guillen-Gosalbez, 2008), product and volume (Sahinidis & Grossmann, 1991), (Norton & Grossmann, 1994), (Bok, Grossmann, & Park 2000), and (Neiro & Pinto, 2004), and process (Swaney & Grossmann, 1985), (Grossmann & Floudas, 1987), and (Pistikopoulos & Grossmann, 1988). The definition of each flexibility type is given in Table 1-2.

Table 1-2 Types of flexibility and their definition

Flexibility	Definition
Recipe (Ferrer-Nadal et al., 2008)	The ability to have a set of adaptable recipes that can control the process output
Product (Beach et al., 2000)	The ability to change over to produce a new (set of) product(s) economically
Volume (Beach et al., 2000)	The ability to operate a system profitably at different production volumes
Process (Ierapetritou, 2001)	Capability of the process to operate feasibly under changing conditions

1.4.3.1 Recipe flexibility

The flexible recipe concept was originally introduced as a set of adaptable recipes that can control the process output and can be modified to confront any deviation from nominal conditions (Ferrer-Nadal, Puigjaner, & Guillen-Gosalbez, 2008). Recipes specify products and prescribe how products are to be produced. The nominal recipe for a given product represents the optimal compromise between quality and costs. According to the production scenario, recipes can be changed or modified. Verwater-Lukszo (1998) developed this basic idea and introduced the concept of the flexible recipe as a way of systematically adjusting control recipes during the execution of production tasks with the aim to enable the process to perform under different operating conditions. These changing operating conditions may include different feedstock properties, changes in quality specifications, variations in process behavior, new market conditions, other real-world experiences with the process, and so on, none of which is reflected in the recipes, though it would often be profitable to be able to adapt them to the changed conditions.

One of the first attempts to do so was made by Romero, Espuna, Friedler, and Puigjaner (2003) who extended the flexible recipe approach to a plant-wide scheduling problem. Another study was carried out by Ferrer-Nadal, Puigjaner, and Guillen-Gosalbez (2008) who aimed to optimize production scheduling in a batch plant where flexible recipes were used. They integrated a linear flexible recipe model into a multi-purpose batch-process scheduling formulation which enabled integration between a recipe optimization procedure at the control level and a batch-plant optimization strategy. Laflamme-Mayer (2009) developed an SC planning model that exploits the capability of a market pulp mill to use different recipes in a flexible manner to provide adequate support for cost-effective fiber supply use.

1.4.3.2 Product/Volume flexibility

Product flexibility, according to Browne, Dubois, Rathmill, Sethi, and Stecke (1984), is the ability to change over to produce a new product economically and quickly. This definition is consistent with the concept introduced by Sahinidis and Grossmann (1991) and is referred to as flexible production, which addresses the capability of a manufacturing system to produce different products at different times via different production modes. This type of flexibility is generally used in conjunction with volume flexibility, which is the capability of a facility to operate at different production rates. Examples of such flexible facilities include pulp and paper mills which can produce different grades of pulp and paper, or refineries that process different types of crude oil at different volumes (Bok, Grossmann, & Park, 2000). According to Sahinidis and Grossmann (1991), a flexible process network consists of dedicated and flexible production facilities that can be interconnected in an arbitrary manner. Dedicated production facilities manufacture fixed amounts of a set of high-volume products at all times, while flexible production facilities, which are normally used for producing low-volume products, manufacture different products at different times.

One of the first studies in this context is carried out by Sahinidis and Grossmann (1991). They address a network of existing and potential processes and chemicals. The processes can be dedicated or flexible, continuous or batch. Given a forecast of prices and demands, as well as investment and operating costs over a specific time horizon, the objective is to determine capacity expansion and shutdown policy for existing processes, selection of new processes and their capacity expansion policy, production profiles, and sales and purchases of chemicals at each time period. The objective function is the NPV which must be maximized. This work is continued by Norton and Grossmann (1994), who also considered flexibility in raw materials. In this study, processes with potential flexibility on either the feedstock or the product side, as well as processes with flexibility on both sides, are considered. These two studies were dedicated to long-term planning problems. In a more recent study, Bok, Grossmann, and Park (2000) address detailed operational decisions in continuous flexible process networks. The model presented in this study extends previous models by incorporating an inventory profile, changeover costs, intermittent supplies, and production shortfalls. As mentioned earlier, this approach is widely used in refineries and the petrochemical industry. Petrochemical complexes are able to produce several products by means of processes which can operate over a range of production rates. Neiro and Pinto (2004) and Schulz, Diaz, and Bandoni (2005) describe SC planning in petrochemical complexes which use this strategy. Mendez, Grossmann, Harjunkoski, and Kaboré (2006) explained the scheduling of oil-refinery operations, in which continuous processes produce a set of components at constant flowrates and then a blending process is used to transform these components into different derivatives in varying amounts.

1.4.3.3 Process flexibility

From a generic point of view, process flexibility is a property of process operability. Grossmann, Halemane, and Swaney (1983) break down operability into a set of properties such as flexibility, controllability, reliability, and safety. Flexibility is concerned with the problem of ensuring feasible operation of a plant over a whole range of conditions in both steady-state and dynamic environments, while controllability signifies the ability of a plant to move efficiently from one operating point to another as well as to deal efficiently with disturbances (Bahri, Bandoni, & Romagnoli, 1996). Reliability denotes the capability of the process to withstand mechanical and electrical failures, and safety is the prevention of major hazards given possible failures. It is worth noting that this definition of process flexibility is too broad and causes overlaps. For instance, volume flexibility which is the ability of a system to operate on a range of throughputs can also be interpreted as process flexibility.

Grossmann, Halemane, and Swaney (1983) mentioned the need for accounting operability considerations, mainly related to flexibility and controllability, at the design stage. Blanco and Bandoni (2003) named three major approaches to the design-for-operability problem:

- Heuristics: Heuristics rely on rules of thumb. Such recipes can be found in Douglas's famous book on conceptual design (Douglas, 1988).

- Operability measures: Operability measures have been widely used in both open-loop and closed-loop controllability. They describe specific operability features and are used to screen or classify different designs with respect to a particular operability issue. Controllability and resiliency indices such as RGA, NI, DCLI, and SVD are examples of these indices (Blanco and Bandoni, 2003).

- Complete integration: This approach implies the integration between process design and process operability by including operability elements within the process design formulation. This approach takes advantage of multi-objective optimization and can be seen in the works of Grossmann and Pistikopoulos. Pistikopoulos and Grossmann (1988) addressed a stochastic flexibility problem in which the major issue is to determine the appropriate tradeoff between the investment cost for the retrofit design of a system and the expected revenue that will result from having increased flexibility. For this purpose, a number of redesign alternatives with specified degrees of flexibility were obtained from a tradeoff curve which related retrofit cost to flexibility. Then, for these designs, the corresponding expected optimal revenue was evaluated using a modified Cartesian integration method. Pistikopoulos and Grossmann (1989) extended this work for nonlinear models.

1.4.4 Critical analysis

Today's market is subject to huge volatilities in terms of price and demand. The price of oil, fuels, and chemicals, as well as the price of forestry products, change constantly. The demand for some products is not always certain, and sometimes, despite strong demand, the price is too low for the production of a product to be profitable. On the feedstock side, uncertainty exists in terms of price and availability. A forestry company might be obliged to procure its feedstock from different sources over different distances and with different prices. Short product life cycles and increasing competition among companies reveal new uncertainties and risks for different industries (Schiltknecht & Reimann, 2009). To mitigate risks in the face of such uncertainties, it is of crucial importance to enhance adaptiveness and reactivity on one hand and proactivity on the other hand (Schiltknecht & Reimann, 2009). These capabilities are generally called flexibility.

An FBR would be exposed to this kind of volatile environment and would face these risks and uncertainties. Hence, flexibility, of any possible type, must be exploited in an FBR to mitigate risks. An FBR will be able to produce several products, including P&P products, bioproducts, and energy. Producing several products implies the opportunity to take advantage of flexibility, i.e., producing different products at different volumes in different time periods. In a volatile market, depending on feedstock and product prices as well as supply and demand, flexibility can be exploited, and the mill can produce different products in different amounts to optimize and secure the company's margin. The company should analyze its access to feedstock, product prices, and received as well as forecasted demands and find the best alignment between these demands and its production capacity to maximize the company's profit. Moreover, experts believe that feedstock flexibility is a promising element in the success of the FBR. Biorefinery processes, especially thermochemical processes, can accept a wide range of feedstocks. This makes it possible to keep operations running with different types of feedstock and to have the flexibility of procuring feedstock from different sources. It will also be a competitive advantage for the company in the volatile feedstock market, where it must deal with several considerations such as feedstock price, competition from other businesses, sufficient availability, handling, proximity, seasonality, and collection. Therefore, feedstock flexibility is another dimension that can be addressed.

Given that, manufacturing flexibility in FBR is the ability of producing several bioproducts (*Product flexibility*) with different production rates (*Volume flexibility*) in different time periods based on the product price and demand. From a techno-economic point of view, the manufacturing flexibility implies a justifiable increase in the capital cost for the biorefinery that is adequately compensated with the ability of the process to manufacture with flexibility, such that expected volatility in market conditions can be mitigated.

As discussed in the previous section, margins-based operating policy maximizes profit by exploiting the flexibility at the operational level throughout the SC in order to mitigate the risks of market volatility. This flexibility includes product, volume and feedstock flexibility. Therefore, two points with regards to flexibility design must be addressed; the first point is that design issues related to these dimensions of flexibility, i.e. set of products to produce, the operating window of processes, type and availability of feedstock, must be addressed at the strategic level of SC design so that the SC can have a proper performance at the operational level. In other words, the system must be designed in a way that leads to an appropriate performance at the operational level. The second point is that, as margins-based policy has an integrated vision towards the SC, the effect of design decisions must be studied over the entire SC. In other words, design activities related to each node of the SC must not be carried out separately. An SC is a unified entity and the design of each node is directly related to the design of other nodes. Thus, targeting the level of process flexibility must be carried out considering its impact on all SC activities at the operational level. This issue has not been addressed yet.

1.5 Key issues in strategic supply chain design

In the strategic design of an SC, long-term decisions should be made. Such decisions include the type of products that should be produced, the technologies that should be used, the number, location and capacity of each type of facility, e.g., plants, warehouses and distribution centers, as well as the target markets, type of contracts and partnerships to make.

Although such decisions are strategic long-term decisions, they have a direct effect on the operational level activities and the day-to-day business. Treating the SC design and strategic planning separately from short-term scheduling will result in inefficient solution at the operational level (Sousa, Shah, & Papageorgiou, 2008). There exist abundant trade-offs between decisions made at different nodes of the SC because of the interdependencies between different levels of the SC (Maravelias & Sung, 2009). Therefore, there should be integration and coordination between strategic long-term and operational short-term decisions (Grossmann, 2005).

Another important point in making strategic decisions is the consideration of uncertainty. The major uncertainty related to the long term decisions is market uncertainty including price and demand of products (Jung, Blau, Pekny, Reklaitis, & Eversdyk, 2004). There is a need for practices which are able to identify major uncertainties about the firm's future. Such practices help senior management in developing effective contingency plans and hedging strategies for coping with them (Shapiro, 2004).

In this section, the two abovementioned key issues in strategic SC design, i.e. integrated approaches for SC design and uncertainty in SC design, are reviewed.

1.5.1 Integrated supply chain design and planning

In the context of process design, reflecting the operational issues of a process into its design has been widely studied. Two-stage stochastic programming formulation is often used in such studies. Ierapetritou and Pistikopoulos (1995) present an approach for optimal process design whose objective is to determine the design that maximizes expected revenue or profit while simultaneously measuring design feasibility. Thomaidis and Pistikopoulos (1995) introduce a method for integrating maintenance and safety aspects in the operability analysis of process systems using a stochastic process model that reflects random process variations, equipment, failures and/or malfunctions, external unexpected events into the design problem. Cheng, Subrahmanian, and Westerberg (2005) develop a model for the simultaneous consideration of upper-level design and lower-level production decisions.

This approach has also got attention in SC design research. Sabri and Beamon (2000) develop a mathematical formulation which combines strategic and operational design and planning decisions using an iterative solution procedure. Designing integrated logistics models for locating production/distribution facilities in a multi-echelon environment needs two fundamental decisions; strategic, i.e. where to locate plants and warehouses, and operational, i.e. production and distribution strategy from plants to warehouses to customers. Jayaraman and Pirkul (2001) develop an integrated production and distribution design problem from a strategic perspective whose goal is to evaluate the expansion, contraction or relocation of facilities in a network and their associated production tasks and unique customer assignments to each facility. The model can also be used at the planning and scheduling setting to assign the production and distribution tasks to existing facilities. Maravelias and Grossmann (2001) address the simultaneous optimization of scheduling activities in new product development and design/planning of batch manufacturing facilities using an MILP. Kallrath (2002b) introduces a simultaneous strategic and operational planning in a multi-site production network, whose long-term objectives are minor changes to the infrastructure (e.g. addition and removal of equipment from sites) and raw material purchases and contracts, while operational decisions include operating modes of equipment in each time period, as well as production and supply of products. Jang, Jang, Chang, and Park (2002) present a SC network management system which integrates four key activities. It involves four modules; supply network design optimization module, planning module for production and distribution operations from raw material suppliers to customers, model management module, and data management module. Goetschalckx, Vidal, and Dogan (2002) address the potential savings created by the integration of the design of strategic global SC networks with the determination of tactical production-distribution allocations and transfer prices. They develop two models; the first one focuses on the setting of transfer prices in a global SC in order to maximize the after-tax profit of an international corporation, while the second model focuses on the production and distribution allocation in a single country system. Sousa, Shah, and Papageorgiou (2008) develop a two-stage model for making strategic and operational decisions. In the first stage, the global SC network is redesigned and the production and distribution plan optimized. The output decisions from the first stage including the SC configuration and allocation decisions are employed as the input parameters for the second stage to model a short-term operational task, which is used to test the accuracy of the derived design and plan. The outputs of this stage determine the detailed production and distribution plans as well as the customer service level.

Grossmann (2005) categorizes the mathematical approaches for solving such problems into two groups; simultaneous optimization over a common time grid, and decomposition techniques for integrating two different levels. The first approach results in a very large-scale multi-period optimization model, because the lower-level variables have to be elevated to the upper level. Aggregation and decomposition strategies can be applied to alleviate the burden of solving such large problems. On the other side, decomposition techniques, as discussed in section 1.1.2.3, divide the problem into two sub-problems, where the upper-level problem is the aggregation of lower-level problem

1.5.2 Uncertainty in supply chain design

Shapiro argues three related methodologies for considering uncertainty at the design stage: scenario planning, stochastic programming, and risk management (Shapiro, 2004), the two formers have been widely applied by the researchers. Scenario planning is a deterministic way of addressing uncertainty. As stated by Schoemaker (1993) “Scenarios are defined as focused descriptions of fundamentally different futures presented in coherent narratives.” Thus, scenario planning can be interpreted as an implicit way of addressing uncertainty. On other side, stochastic programming models the uncertainties associated with several scenarios in an explicit way. The distinction between deterministic and stochastic programming models is that, in a deterministic scenario planning model, the system is optimized for all scenarios separately as if they will occur with certainty. On the contrary, a stochastic model considers all scenarios, each with an associated probability of occurrence, as a probabilistic description of the future (Shapiro, 2004).

1.5.2.1 Scenario-based supply chain design

Scenario planning, as a methodology for strategic planning, has been used for designing the SCs. This approach has got more attention in industry more than it has in academia. Managers have been introduced to the deterministic approach, which is less complicated (Shapiro, 2004). But in academia, it got less attention compared to the stochastic approach. Iyer and Grossmann (1998) introduce a model which determines the optimal selection and expansion of processes over a long-range planning horizon, incorporating uncertainty in terms of demands and prices of chemicals by utilizing multiple scenarios for varying situation. Salema, Barbosa-Povoa, and Novais (2007) present a scenario-based approach for general closed-loop SCs that incorporates facility capacity limits, multi-product and uncertainty on products demands and returns.

1.5.2.2 Stochastic approach for supply chain design

The major approach for addressing uncertainty is the stochastic programming. In stochastic programming, the problem is divided into a number of stages. Some uncertain parameters are revealed between each stage and the decision maker must choose an action that optimizes the current objective plus the expectation of the future objectives. The most common stochastic programs are two-stage models that are solved using Benders' decomposition techniques (Grossmann, 2005).

Tsiakis et al. (2001) develop a multi-period model that captures demand uncertainty through a scenario tree, where each scenario represents a different discrete future outcome. The model considers flexible production capacity which must be allocated among different products. Ahmed and Sahinidis (2003) introduce a multi-stage stochastic capacity expansion integer program where scenarios are used to explicitly define uncertainties in the problem parameters. Guillen, Mele, Bagajewicz, Espuna, and Puigjaner (2005) propose a multi-objective multi-scenario stochastic MILP model for the design/retrofit of SCs, which maximizes profit and customer satisfaction and minimizes financial risk. Another study in the field of SC design under demand uncertainty is carried out by Guillen, Mele, Espuna, and Puigjaner (2006) utilizing a multi-stage stochastic programming approach that integrates strategic and tactical/operational levels. Puigjaner and Lainez (2008) propose an enterprise-wide model considering uncertainty and process dynamics, which also contemplates cross-functional decisions. The model comprises f a design-planning and a financial formulation. Moreover, a model predictive control (MPC) methodology is proposed that includes a stochastic optimization approach, employing a scenario-based multi-stage stochastic MILP model to predict process output over the long term. Guillén-Gosálbez and Grossmann (2009) address the optimal design and planning of sustainable chemical SCs under uncertainty in the life cycle inventory associated with the network operation, using a bi-criterion stochastic MINLP which accounts for both NPV and environmental performance of the network through Eco-indicator 99, which included recent advances made in LCA. You and Grossmann (2010) propose a model for the optimal design of a multi-echelon SC and the associated inventory systems in the presence of uncertain customer demands. Using a multi-echelon stochastic model for inventory system, the model simultaneously determines the transportation, inventory, and network structure of a multi-echelon SC.

1.5.3 Critical analysis

As discussed in section 1.2 of the literature review, in order to be able to apply a margins-based policy, the flexibility of the system must be designed, on one side, considering the operational issues, and on the other side, considering the linkage between all SC nodes. Designing the flexibility is a part of SC design, because processes are the heart of the SC. Given that, an integrated approach, aggregating strategic, tactical and operational issues, is required for the SC design and for the design of flexibility of processes as parts of the SC, in order to reflect the operational issues at the strategic level. More specifically, for targeting the level of flexibility, having operational (not necessarily scheduling) information on the production volume and its variations is of crucial importance. The operational profit associated with each level of flexibility helps estimating the profitability of that level. In this regard, calculating the capital cost of each flexibility level is critical. Moreover, as uncertainty is associated with market price and demand, uncertainty must be addressed in the SC design and its flexibility so that SC has a robust performance in the short term.

In order to address practical problems in the biorefinery context, the reality of this industry must be taken into account. SC studies in this context address some critical issues related to the reality of the industry, however, by applying the holistic approaches, i.e. developing large mathematical formulations for solving such problems. There is a lack of an approach that addresses real problems by considering the options that a company has in terms of market, feedstock, process, partnership, etc. Such an approach simplifies the problems and makes the results more interpretable for industry.

1.6 Supply chain capacity expansion planning

As mentioned earlier, one of the decisions to make at the strategic level is concerned with the set of products that must be produced and the set of processes/technologies that must be installed and employed. In this regards, a sub-problem of SC strategic design is related to long-term capacity planning. Given the initial processes and their capacities, the goal of the problem is to determine which processes to operate in the future (chosen from a candidate set) and where and when to expand capacity (Shah, 2005).

Going through the literature on capacity-expansion planning, it can be seen that two types of problems have been addressed in this context; deterministic and stochastic (Oh & Karimi, 2004). Deterministic problems suppose fixed parameters over a given planning horizon, while stochastic problems allow uncertainty in some parameters. Oh and Karimi (2004) made a comprehensive review on the capacity-expansion planning literature. Another classification is based on the approach taken for capacity-expansion planning. Some researchers consider all variables and factors of the problem in one large mathematical and optimization formulation, whereas some others develop systematic methodologies in which optimization is a part of the entire framework.

1.6.1 Mathematical formulations for capacity-expansion planning

One of the earliest studies in this field is carried out by Sahinidis, Grossmann, Fornari, and Chathrathi (1989). They propose a multi-period MILP model which, considering the forecasts of prices and demands of the chemicals over a long planning horizon, determines new processes, expansion plans, and shutdown policies to maximize the NPV of a project. Sahinidis and Grossmann (1992) improve the solution efficiency of such problems. Li and Tirupati (1994) introduce a capacity expansion planning model which selects technology types (flexible versus dedicated facilities). Liu and Sahinidis (1996) solve address uncertainty by including product demand scenarios in each time period in the capacity expansion planning problem. They use projection techniques for solving this class of stochastic problems. Iyer and Grossmann (1998) solve the same problem by decomposition and iteration. Ahmed and Sahinidis (1998) introduce robustness into capacity expansion planning models by penalizing the downside risk defined as the costs above the expected cost. Applequist, Pekny, and Reklaitis (2000) consider risk mitigation along with optimizing the expected return, by introducing the concept of a risk premium. For an investment plan regarding capacity expansion to be chosen, it should at least meet the risk premium. Lee et al. (2000) present an MINLP which integrates capacity expansion planning with production-distribution considerations. Papageorgiou, Rotstein, and Shah (2001) develop a multi-period MILP model for managing product portfolios in the pharmaceutical industry, considering product development and introduction along with capacity planning. They take a deterministic approach for capacity planning by assuming pre-specified sizes and costs for every possible expansion or new facility construction. Maravelias and Grossmann (2001) apply a two-stage stochastic optimization approach for scheduling the regulatory tests for new products along with production and capacity-expansion planning of batch plants under the uncertainty associated with the outcomes of such regulatory tests. Naraharisetti, Karimi, and Srinivasan (2008b) develop a large MILP model for facility location, relocation, investment, disinvestment, technology upgrade, production-allocation, distribution, supply contracts, capital generation, etc, considering disinvestment, technology upgrade, material supply contracts, and loans and bonds for capital generation, while including strategic asset management and tactical planning, capacity planning, financial/regulatory factors, and production–distribution.

1.6.2 Systematic design methodologies for long-term planning

Cheng et al. (2003) work on a "design/investment under uncertainty" problem. They propose a Markov decision process with recourse that can be used for decision making throughout the process life cycle and at different hierarchical levels and can consider uncertainties associated with market conditions and technology evolution. It provides multiple criteria such as expected profit, expected downside risk, and process lifetime. The formulation incorporates design decisions and future planning by explicitly integrating both upper-level investment decisions and lower-level production decisions as a two-stage optimization problem. The output is Pareto optimal design strategies. The process starts by selecting conflicting objectives such as expected profit and expected downside risk by the decision makers. Then, a dynamic process design is formulated, which integrates the design decisions to planning activities in each time period. The formulation considers different uncertainties, e.g. product price and demand, as well as technology improvements. Finally, using a multi-objective stochastic dynamic model set of Pareto optimal solutions are obtained.

Oh and Karimi (2004) propose a four-prong approach as a strategic decision making tool for capacity expansion planning in multinational companies. The approach starts by introducing and classifying key regulatory factors that can affect the earnings or business operations. Then, a deterministic capacity-expansion-planning model, whose goal is to determine sizes of expansions or new facilities, is used. Finally, an extended version of the deterministic model is employed to address important aspects such as distribution centers, outsourcing, and uncertainty in problem parameters. In this way, the importance and effect of incorporating multiple regulatory factors in capacity-expansion-planning models can be demonstrated. Sammons, Eden, Yuan, Cullinan, and Aksoy (2008) propose a general systematic framework for optimizing product portfolio and process configuration in integrated biorefineries. The framework first determines the variable costs as well as fixed costs using data in terms of yield, conversion and energy usage for each process model. Next, process integration tools, e.g. pinch analysis, are employed to optimize process models by reducing energy usage, material consumption, and waste stream. Finally, the optimized model generates data for economic metrics and environmental performance measures. An optimization formulation enables the framework to decide whether a certain product should be sold or processed further, or which processing route to pursue if multiple production pathways exist for a special product. However, this methodology does not involve market investigations before selecting the products and no SC metric is considered in the framework. Sharma, Sarker, and Romagnoli (2011) develop a strategic decision analysis framework for technology and product portfolio design for a multi-product multi-platform biorefining enterprise. The framework considers the operational, economic, environmental and social aspects of a project by utilizing flexibility, structural evaluation, environmental LCA and social LCA modules. An MILP financial planning model is used with the objective of maximizing the stakeholder value by selecting appropriate feedstocks, technologies, and products.

1.6.3 Critical analysis

Implementing new processes and technologies and their capacity expansion strategy is associated with risk and uncertainty. Moreover, such radical changes are structural and related to the entire SC. Therefore, different tools must be used to analyze the performance of a specific project in future. Several scenarios must be considered for the future. Advanced mathematical programming techniques enable addressing different aspects of a project, though they are commonly large and complex. Managers must take into consideration several aspects of a future plan and see its future in different possible conditions. Thus, it is of crucial significance that analysis tools are developed in a way that convince industrial people that, on one hand, they are able to address different sides of a future investment, and on the other hand, they are not too complicated to be used in practice.

1.7 Gaps in the body of knowledge

Based on the literature review the following gaps in the body of knowledge were identified:

Biorefinery operating policy: Margins-based approach

There is no study on the operating policy of biorefinery SC, which clearly illustrates (1) the importance of a profit-oriented approach versus cost-minimization thinking, (2) the implication of taking advantage of the inherent flexibility of biorefinery processes and biorefinery SC, and (3) the significance of considering all SC nodes in analyzing the profitability of a system. All studies have taken such concepts for granted.

Metrics for evaluating the SC performance

Metrics of robustness mainly considers an average deviation and variance from a base-case desired value. There is a need for a metric that takes into account the number of downside variations. Furthermore, no metric of flexibility has been proposed yet that addresses volume flexibility and can be used in designing and analyzing process alternatives. Lastly, the link between the two metrics, their effect on profit and profitability, and the fact that how profitability and robustness change with flexibility have not been studied at the design stage.

Design for flexibility: Targeting the level of flexibility via a SC-based analysis

All previous analyses which considered the linkage between flexibility and SC issues, have examined the exploitation of flexibility at the tactical/operational level. In other words, SC analysis has been used to determine how the flexibility of a system must be managed at the tactical level and be exploited at the operational level. This linkage between flexibility and SC issues has never been made at the design level for designing or targeting the design of flexibility. The main approach for designing or targeting the design of flexibility has been a trade-off between flexibility and the cost of having flexibility. This cost implies either the cost of modifications needed for retrofit design, or the cost associated with a higher flexibility for a Greenfield design, and thus, no integration with SC costs has been considered. Therefore, to our knowledge, no study has brought up a SC analysis to the design stage to reflect, not only process-related costs, but also SC-related costs in designing or targeting the design of process flexibility.

Supply chain strategic design: A scenario-based approach

In the biorefinery context, the SC literature took the holistic approach in SC design, i.e. developing a generic mathematical formulation which calculates the value of a very large number of design and operational decision variables. But there is no systematic methodology for the strategic design of biorefinery SC that takes into account the vision of a specific company by defining scenarios-alternatives, addresses practical issues such as partnership, and makes decision in a step-wise manner, which more suits the industrial approach.

Capacity expansion planning: A systematic methodology for phased implementation approach

There is no design methodology proposed in the biorefinery literature that makes a proper linkage with other analysis tools such as product portfolio definition and techno-economic studies, integrates flexibility design (targeting the level of flexibility) and SC network design, analyzes several strategies which are implemented through phases considering the company's perspective, and provides metrics to be used for further decision making in an MCDM framework.

CHAPTER 2 OVERALL METHODOLOGICAL APPROACH

In this section, first the philosophy behind the methodology is explained. Next, the SC mathematical formulation is presented and the case study is introduced. Finally, the methodology is presented.

2.1 Supply chain-based analysis: A bottom-up approach

As mentioned in the definition of the margins-based policy, the ultimate goal of this policy is to maximize profit across the entire SC. In fact, the margins-based operating policy exploits system's flexibility, i.e. the ability of producing different products with different volumes in different time periods, at the operational level to maximize the margins. Thus, an SC-based analysis is needed to show how the flexibility should be managed and exploited at the operational level to maximize SC profit. Moreover, at the process design level, flexibility must be designed in a way that ensures the best performance at the operational level and the SC profit maximization. Hence, SC profitability must be reflected at the process design stage. On the other hand, from a SC network design perspective, SC network must be designed so that it enables margins-based operating policy to exploit flexibility. In other words, the SC network should be designed in such a way that the maximum exploitation of flexibility can be obtained. Therefore, an SC-based analysis is required to address two aspects: operational and design. That being said, the challenge is to develop a SC-based analysis which can be used:

- At the design stage, to reflect SC profitability as a design metric in targeting the design of flexibility and in SC network designs, and
- At the tactical-operational level, to improve SC profitability by exploiting flexibility.

Figure 2-1 provides a schematic illustration of the linkage between SC analysis, and design and operational decisions. The bottom-up approach shows the importance of operational-level information for design-related decisions and implies that such information should be brought up to the strategic-level decision-making to obtain a system with greater flexibility in its performance. Considering this bottom-up approach, an SC-based methodology can be developed to enable decision-makers to define and to analyze various biorefinery options from an SC perspective and to evaluate their implementation strategy under different market conditions based on the effects of the design of each option on its operational performance.

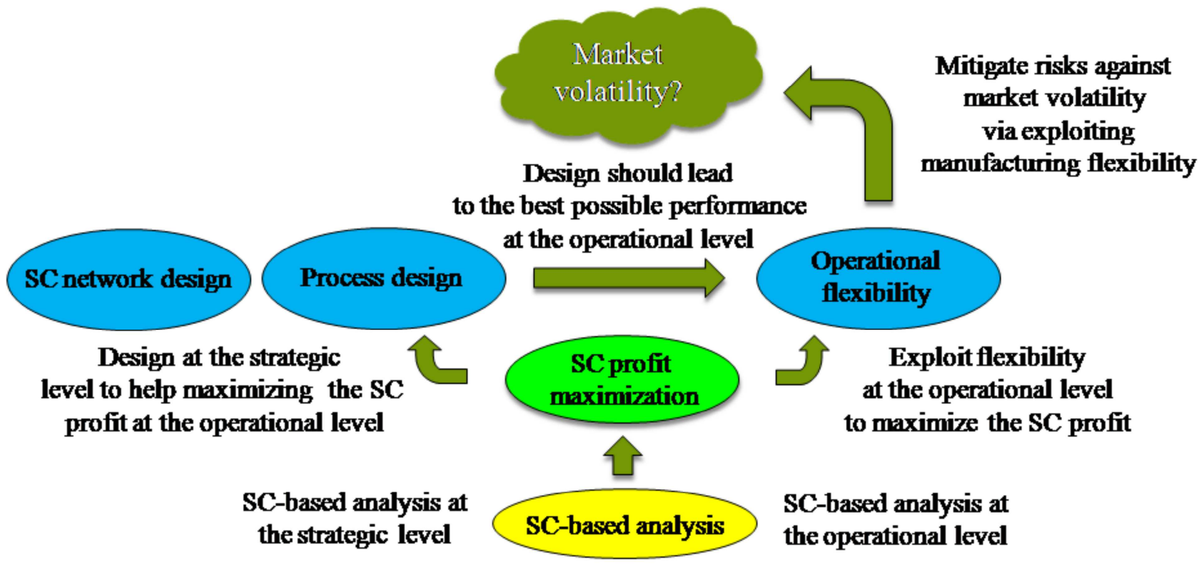


Figure 2-1 Linkage between SC-based analysis and design/operational decisions

2.2 Project methodology

As mentioned earlier, the major objectives of this work are defining biorefinery options including product/process portfolios with targeted level of flexibility, designed SC network and defined implementation strategy. All these decisions are made based on the SC performance of biorefinery. Therefore, an SC mathematical tool is required as a major tool in the methodology. Moreover, before getting to the design stage, the appropriate operating policy of the biorefinery must be identified, so that the design is executed based on the operating policy. Next, the relevant metrics for design activities must be developed to help designing a flexible system against market volatility. After developing the SC mathematical formulation, identifying the right operating policy, and introducing relevant metrics for design activities, the SC design methodology for targeting the level of flexibility, SC network design and defining the implementation strategy can be developed. Figure 2-2 illustrates the project methodology of this thesis. Project methodology starts with developing an SC mathematical formulation for optimizing the Sc activities. This formulation will be used in different steps of the SC design methodology. Then, the value of margins-based policy versus the manufacturing-centric approach is illustrated. Afterwards, relevant performance metrics for design and analysis purposes are introduced. Finally, a step-wise SC design methodology is developed.

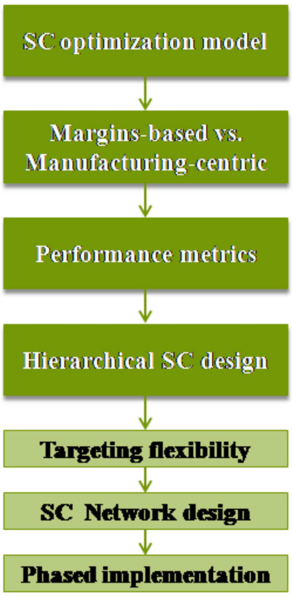


Figure 2-2 Project methodology

A major tool required by this methodology is an SC mathematical formulation which is presented in the next section.

2.3 Supply chain mathematical formulation

In this thesis, SC mathematical formulation is used to show the value of margins-based policy and the performance metrics, and also the SC performance of different biorefinery options, including product/process portfolios with different levels of flexibility and SC network configurations, and their implementation strategy.

The SC framework presented in this work aims at maximizing profit across the entire SC by identifying the trade-offs between demand and production capabilities, and by finding the optimal alignment of manufacturing capacity and market demand. The SC optimization framework considers feedstock price and availability, production costs, inventory and delivery costs, as well as product price and demand. Taking this information into account, the SC optimization framework exploits the potential for flexibility and determines which orders must be fulfilled, and therefore, how much of each product must be produced, how they should be stored, and how they should be delivered to maximize SC profit.

On one hand, it is desirable to account for tactical and operational issues at the strategic design level. On the other hand, for design purposes, it is not necessary to go down to too much details, as can be provided by scheduling models. For this reason, the SC framework that is presented in this work is inspired by the tactical model developed for the chemical industry by Kanegiesser (2008). This model is a tactical model that has some operational components. The model divides each time period into several hours that can be dedicated to production, changeover and maintenance. In this way, a better cost representation can be made by the model.

The SC framework is formulated as a multi-period optimization problem aiming at profit maximization. The framework is generic and, depending on the way parameters including feedstock, products, and processes are defined for it, it can be used for any case study. For this specific study, the framework is used for biorefinery processes. Later in this section some specificities of the model related to biorefinery processes are explained. The SC framework considers the management of a multi-product, multi-echelon SC, including existing production and warehousing facilities, feedstock suppliers, as well as a number of customer zones. Different types of feedstock are provided by several suppliers. Production facilities can make one or several products. Processes are either dedicated, i.e. they produce only one product, or flexible from a product perspective, i.e. they are able to produce several products through different production modes or "recipes". In other words, a flexible process can use different recipes to produce different products in different production modes. Changing from one recipe to another incurs changeover cost and time. Processes can be idled or shutdown for scheduled maintenance. The steam required for each process is provided by both fuel and other sources inside the process, e.g. biomass. Warehouses can receive material, either feedstock or product, from different sources and plants, and supply different markets. Each market places order in two ways: by contract, i.e., for the long term, and on the spot market, i.e., for the short term. In case of a contract, specific quantities of products must be delivered to the customer in specific time periods. In other words, the contractual orders must be either fulfilled up to a certain pre-specified level, or be declined. The spot demand can be partially/completely fulfilled or declined. Transportation routes link suppliers, facilities and customers together. The model is formulated as an MILP problem with a discrete time horizon of 48 weeks. Each time period is broken down into hours. Several subsets have been created to link parameters and variables to each other. For instance, processes can only produce certain materials. Each supplier may provide a specific type of feedstock and each customer may need a specific product. Production plants may be able to link with some specific suppliers and markets. This, in general, will reduce the possible options and thus, the complexity of the problem. The main decision variables of the model include:

- Binary variable for contract selection
- Binary variable representing the recipe used on a process. Another binary variable is used to determine whether or not a recipe is used consecutively on a process. This binary variable helps considering the changeovers.
- Amount of material processed and produced by each process
- Flow of materials, i.e. feedstock and product, to and from the mill
- Number of hours taken by each recipe in a specific process
- Amount of energy produced and/or consumed by each process

Some key aspects of the model are as follows:

- The model is run for 48 periods of one week.
- The variables are calculated for each time period.
- The objective function, which is the profit, and all variables are calculated weekly over a year.
- If a contract is accepted, it must be fulfilled over the entire year completely or to a specified level.
- Spot demands can be declined or fulfilled partially/completely.
- Production level can vary between certain boundaries, showing volume flexibility.
- Some processes can produce more than one product using different recipes.
- Only one recipe can be used on a process in each period.
- A recipe can be changed to another recipe between two time periods. That implies a changeover. Changeover time and cost is considered in the formulation.
- To account for time losses during changeovers and shutdowns, each time period is divided into hours.

Some specificities of the model related to biorefinery are as follows:

- Different types of feedstock, e.g. woody biomass, forest residues, agricultural residues, etc., can be defined and their availability from different suppliers can be modeled.

- A recipe links a specific type of feedstock to either an intermediate product or a final product. Each recipe is associated with a specific yield, and thus, can be used to model the yields of different feedstocks to different products.
- Different processes can be defined and their input can come either from outside of the mill or from inside the process. Moreover, there is a representation of a process generating or consuming energy. These two potentials can be used for energy integration purposes. Processes that produce energy, such as boilers, can be defined and their feed can be provided by fuel and excess biomass, e.g. lignin. Then, the energy required by other processes can be provided by the boilers.

Although the model is for operational purposes, it can also be used for design purposes. More specifically, by adding a few numbers of variables, parameters, and constraints, the model can be used as a capacity expansion planning model which considers design and operational variables simultaneously. In the "Future works" section (Chapter 5), some binary variables, parameters, equations and constraints are introduced to evolve this model to a more generic model. The model is presented below:

Nomenclature

Sets

$j \in J$	Supplier locations
$l \in L$	Mill locations
$k \in K$	Sales locations
$p \in P$	Processes
$r \in R$	Recipes
$m \in M$	Materials
$t \in T$	Time

Subsets

Suppliers that can supply mill: Set of $\{j,l\} \in L^{JL} \quad \forall j \in J, l \in L$

Customers that can be served by mill: Set of $\{l,k\} \in L^{LK} \quad \forall l \in L, k \in K$

Processes at mill: Set of $\{l,p\} \in P^{L} \quad \forall l \in L, p \in P$

Recipes available on process: Set of $\{l,p,r\} \in R^{P} \quad \forall \{l,p\} \in P^{L}, r \in R$

Materials offered by suppliers: Set of $\{j,m\} \in M^{J} \quad \forall j \in J, m \in M$

Materials produced/processed at mill: Set of $\{l,m\} \in M^{L} \quad \forall l \in L, m \in M$

Materials requested by customers: Set of $\{k,m\} \in M^{K} \quad \forall k \in K, m \in M$

Input materials of a process: Set of $\{l,p,m\} \in M^{P-in} \quad \forall \{l,p\} \in P^{L}, m \in M$

Output materials of a process: Set of $\{l,p,m\} \in M^{P-out} \quad \forall \{l,p\} \in P^{L}, m \in M$

Input materials of a recipe: Set of $\{l,p,r,m\} \in M^{R-in} \quad \forall \{l,p,r\} \in R^{P}, m \in M$

Output materials of a recipe: Set of $\{l,p,r,m\} \in M^{R-out} \quad \forall \{l,p,r\} \in R^{P}, m \in M$

Constructed Subsets

Materials that can be transported between a supplier and a mill:

$\{j,l,m\} \in M^{JL} \quad \forall \{j,l\} \in L^{JL}, \{j,m\} \in M^{J}, \{l,m\} \in M^{L}$

Materials that can be transported between a mill and a customer:

$\{l,k,m\} \in M^{LK} \quad \forall \{l,k\} \in L^{LK}, \{l,m\} \in M^{L}, \{k,m\} \in M^{K}$

Parameters

a_{lprm}^{input}	Recipe material conversion Input factor of material *m* when using recipe *r* on process *p* in mill *l* (dependent on throughput)
a_{lprm}^{output}	Output factor of material *m* when using recipe *r* on process *p* in mill *l*
$b_{lpr}^{input-steam}$	Steam consumption factor for recipe *r* in process *p* in mill *l*
$b_{lpr}^{output-steam}$	Steam production factor for recipe *r* in process *p* in mill *l*

$b_{lpr}^{input-elect}$	Electricity consumption factor for recipe *r* in process *p* in mill *l*
$b_{lpr}^{output-elect}$	Electricity production factor for recipe *r* in process *p* in mill *l*
$c_{lpr}^{proc-var}$	Variable operating cost of using recipe *r* on process *p* in mill *l*
$c_{lt}^{mill-fix}$	Fixed operating cost at mill *l* during time period *t*
$c_{jlm}^{transport-sup}$	Transportation cost of material *m* from supplier *j* to mill *l*
$c_{lkm}^{transport-sale}$	Transportation cost of material *m* from mill *l* to a customer *k*
c_{lm}^{stor}	Storage cost of material *m* in mill *l*
$c_{lp}^{shutdown}$	Shutdown cost of process *p* in mill *l*
$c_{lp}^{changeover}$	Changeover cost of process *p* in mill *l*
c_{lt}^{elect}	Electricity cost / selling price at mill *l* during time period *t*
c_{kmt}^{sales}	Selling price of product *m* to customer *k* during time period *t*
c_{jmt}^{sup}	Purchasing price of a feedstock *m* from supplier *j* during time period *t*
$c_{kmt}^{salescost}$	Sales cost for product *m* sold to customer *k* during time period *t*
H_{lpr}^{camp}	Minimum campaign length (in hour) for recipe *r* in process *p* in mill *l*
$H_{lp}^{changeover}$	Changeover time (in hour) on process *p* in mill *l*
H_{lpt}^{proc}	Available processing hours on process *p* in mill *l* during time period *t*
$\underline{Q}_{lpr}^{proc}$	Minimum throughput (process rate) of recipe *r* on process *p* in mill *l*
$\overline{Q}_{lpr}^{proc}$	Maximum throughput (process rate) of recipe *r* on process *p* in mill *l*
$\underline{Q}_{lm}^{stor}$	Minimum storage quantity of material *m* in mill *l*
$\overline{Q}_{lm}^{stor}$	Maximum storage quantity of material *m* in mill *l*
$\underline{Q}_{jmt}^{supp}$	Minimum supply quantity of material *m* offered by supplier *j* during time period *t*

$\overline{Q}_{jmt}^{supp}$	Maximum supply quantity of material *m* offered by supplier *j* during time period *t*
$\underline{Q}_{kmt}^{sales}$	Minimum quantity of material *m* requested by customer *k* during time period *t*
$\overline{Q}_{kmt}^{sales}$	Maximum quantity of material *m* requested by customer *k* during time period *t*
$\overline{Q}_{jlm}^{transport}$	Maximum transportation quantity of material *m* between supplier *j* and mill *l*
$\overline{Q}_{lkm}^{transport}$	Maximum transportation quantity of material *m* between customer *k* and mill *l*
$S_{lm}^{mat-start}$	Initial storage quantity of material *m* in mill *l* at time 0
$S_{lm}^{mat-end}$	Minimum storage quantity of material *m* in mill *l* at time T
ε_{lpt}^{proc}	Shutdown hours on process *p* in mill *l* during time period *t*
$\alpha_{lpr}^{rec-start}$	Initial recipe *r* on process *p* in mill *l*

Variables

f_{jlmt}^{sup}	Flow of material *m* from supplier *j* to mill *l* during time period *t*
f_{lkmt}^{mill}	Flow of material *m* from mill *l* to mill *l'* during time period *t*
f_{lkmt}^{sales}	Flow of material *m* from mill *l* to customer *k* during time period *t*
h_{lprt}^{rec}	Number of hours spent on recipe *r* on process *p* in mill *l* during time period *t*
S_{lmt}^{mat}	Inventory of material *m* in mill *l* during time period *t*
v_{lpt}^{input}	Input steam quantity on process *p* in mill *l* during time period *t*
v_{lpt}^{output}	Output steam quantity on process *p* in mill *l* during time period *t*
w_{lpt}^{input}	Input electricity quantity on process *p* in mill *l* during time period *t*
w_{lpt}^{output}	Output electricity quantity on process *p* in mill *l* during time period *t*
x_{lmpt}^{proc}	Input quantity of material *m* on process *p* in mill *l* during time period *t*
y_{lmpt}^{proc}	Output quantity of material *m* on process *p* in mill *l* during time period *t*

y_{lprmt}^{rec} Output quantity of material *m* using recipe *r* on process *p* in mill *l* during time period *t*

$y_{lprt}^{rec-tot}$ Total mass output of recipe *r* on process *p* in mill *l* during time period *t*

α_{lprt}^{proc} Selection of recipe *r* on process *p* in mill *l* during time period *t* (binary)

β_{lprt}^{proc} Successive selection of recipe *r* on process *p* in mill *l* during time periods *t* and *t-1* (binary)

θ_{kmt}^{ord} Selection of the order of product *m* from customer *k* during time period *t* (binary)

Objective Function

The objective function is the global net profit of the enterprise to be maximized. This profit consists of revenues from the sales of products and electricity, minus several variable and fixed costs.

$$\max Profit = \begin{pmatrix} Revenues - ElectricityCost - SalesCost \\ -VariableOpCost - FixedOpCost - ChangeoverCost - ShutdownCost \\ -TransportationCost - StorageCost - ProcurementCost \end{pmatrix} \tag{1}$$

Revenues from sales are equal to the flow of materials sent to each customer multiplied by the selling price.

$$Revenue = \sum_{t\in T} \sum_{\{k,m\}\in M^K} f_{lkmt}^{sales} c_{kmt}^{sales} \tag{2}$$

Electricity sales or purchases are function of the production/consumption at the mill. If the mill produces more electricity than needed, then electricity is sold to the grid. Otherwise, it is assumed that it is bought from the grid at the same price.

$$ElectricityCost = \sum_{t\in T} \sum_{\{l,p\}\in P^L} (w_{lpt}^{input} - w_{lpt}^{output}) c_{lt}^{elect} \tag{3}$$

Variable sales costs are customer specific and are a percentage of product prices.

$$SalesCost = \sum_{t\in T} \sum_{\{k,m\}\in M^K} f_{lkmt}^{sales} c_{kmt}^{salescost} \tag{4}$$

Variable operating costs are a function of process throughput such as chemical consumption.

$$VariableOpCost = \sum_{t\in T} \sum_{\{l,p,r\}\in R^P} c_{lpr}^{proc-var} y_{lprt}^{rec-total} \tag{5}$$

Fixed operating costs are calculated at the plant.

$$FixedOpCost = \sum_{t \in T} \sum_{l \in L^{mill}} c_{lt}^{mill-fix} \tag{6}$$

Changeover cost is equal to the number of transitions multiplied by the changeover cost per transition. This cost is not considered sequence dependent.

$$ChangeoverCost = \sum_{t \in T} \sum_{\{l,p,r\} \in R^P} (1 - \sum_{r \in R_p^{proc}} \beta_{lprt}^{proc})\ c_{lp}^{changeover} \tag{7}$$

The shutdown cost of a process is a function of the number of shutdown hours during a time period. Scheduled shutdowns for maintenance are considered here as a hard constraint.

$$ShutdownCost = \sum_{t \in T} \sum_{\{l,p\} \in P^L} \varepsilon_{pt}^{proc} c_{lp}^{shutdown} \tag{8}$$

Transportation cost is calculated by multiplying the amount of material shipped from a source (supplier *j* or mill l) to a sink (mill *l* or customer *k*) and the shipping cost per mass of that route.

$$TransportationCost =$$
$$\sum_{t \in T} \sum_{\{j,l,m\} \in M^{JL}} f_{jlmt}^{sup} c_{jlm}^{transport-sup} + \sum_{t \in T} \sum_{\{l,k,m\} \in M^{LK}} f_{klmt}^{sales} c_{jlm}^{transport-sales} \tag{9}$$

Storage cost in a facility is equal to the amount of material kept in inventory during each time period multiplied by its storage cost per month.

$$StorageCost = \sum_{t \in T} \sum_{\{m,l\} \in M^L} S_{mlt}^{mat} c_{lm}^{stor} \tag{10}$$

Procurement costs are equal to the flow of materials transported from each supplier to different facilities multiplied by the selling price.

$$ProcurementCost = \sum_{t \in T} \sum_{\{j,l,m\} \in M^{JL}} f_{ll'mt}^{sup} c_{lmt}^{sup} \tag{11}$$

Demand and Procurement

Suppliers and customers may offer/request materials between lower and upper fulfilment bounds, as shown in equations 12 and 13. Lower and upper bounds for customers are multiplied by binary variable θ, which is equal to one if the order is fulfilled and equal to zero otherwise. For contractual orders, the lower and upper bounds are equal, because the contractual amount is fixed. But the lower bound for spot orders is equal to zero and the model can determine what percentage of the order should be fulfilled. Equation 14 forces θ of all time periods to be equal to θ of first time period. In this way, if an order is accepted in the first period, it must be fulfilled over all other time periods. This constrain refers to contractual orders, which either must be fulfilled throughout the year, or must be refused. This will not cause any problem for spot orders, which can be fulfilled partially at any time, because if model decides not to fulfil a spot order, model can assign zero to fulfilled amount for this order, as the lower bound for spot order fulfilment is zero, no matter if θ is zero or one. Thus, it can be said that θ is one for all spot orders and can be zero or one for contractual orders.

$$\underline{Q}_{lmt}^{supp} \leq f_{ll'mt}^{sup} \leq \overline{Q}_{lmt}^{supp} \qquad \forall \ \{j,l,m\} \in M^{LJ}, t \in T \tag{12}$$

$$\theta_{ll'mt}^{ord}\underline{Q}_{lmt}^{sales} \leq f_{l'lmt}^{sales} \leq \theta_{ll'mt}^{ord}\overline{Q}_{lmt}^{sales} \qquad \forall \ \{l,k,m\} \in M^{LK}, t \in T \tag{13}$$

$$\theta_{ll'm1}^{ord} = \theta_{ll'mt}^{ord} \qquad \forall \ \{l,k,m\} \in M^{LK}, t > 1 \tag{14}$$

Transportation

A maximum transportation capacity constraint limits the amount of materials that can be transported between locations (suppliers, facilities and customers).

$$f_{jlmt}^{sup} \leq \overline{Q}_{jlm}^{transport-sup} \qquad \forall \ \{j,l,m\} \in M^{LJ}, t \in T \tag{15}$$

$$f_{lkmt}^{mill} \leq \overline{Q}_{lkm}^{transport-sales} \qquad \forall \ \{l,k,m\} \in M^{LK}, t \in T \tag{16}$$

Inventory Management

The material balance at a facility is equal to the previous inventory, plus/minus material coming from and going to other sites as well as the consumption/production from processes.

$$S_{mlt}^{mat} = S_{mlt-1}^{mat} + \sum_{\{j,l,m\}\in M^{JL}} f_{jlmt}^{sup} - \sum_{\{l,k,m\}\in M^{LK}} f_{lkmt}^{sales} + \sum_{\{l,l',m\}\in M^{LL}} f_{ml'lt}^{mill} - \sum_{\{l,l',m\}\in M^{LL}} f_{mll't}^{mill} - \sum_{\{l,p,m\}\in M^{P-out}} x_{lmpt}^{proc} + \sum_{\{l,p,m\}\in M^{P-in}} y_{lmpt}^{proc} \qquad \forall \{l,m\} \in M^{L}, t > 1 \tag{17}$$

At time t=1, S_{mlt-1}^{mat} does not exist and it is replaced by the initial inventory quantity, S_{ml}^{start}.

$$S_{ml1}^{mat} = S_{ml}^{start} + \sum_{\{j,l,m\}\in M^{JL}} f_{jlm1}^{sup} - \sum_{\{l,k,m\}\in M^{LK}} f_{lkm1}^{sales} + \sum_{\{l,l',m\}\in M^{LL}} f_{ml'l1}^{mill} - \sum_{\{l,l',m\}\in M^{LL}} f_{mll'1}^{mill} - \sum_{\{l,p,m\in M^{P-out}\}} x_{lmp1}^{proc} + \sum_{\{l,p,m\}\in M^{P-in}} y_{lmp1}^{proc} \qquad \forall \{l,m\} \in M^{L}, t = 1 \tag{18}$$

To ensure that the optimization model does not completely deplete the inventory at the end of the planning horizon ($t=T$), a constraint specifying the final minimum inventory quantity must be added.

$$S_{mlT}^{mat} \geq S_{ml}^{End} \qquad \forall \{l,m\} \in M^L, t = T \tag{19}$$

Finally, each site has storage capacity constraints.

$$\underline{Q}_{lm}^{stor} \leq S_{lmt}^{mat} \leq \overline{Q}_{lm}^{stor} \qquad \forall \{l,m\} \in M^L, t \in T \tag{20}$$

Recipe selection

Equations 21 to 26 constrain the selection of recipes. Each process has an offline/idle recipe that can be selected for when the process is not needed. Equation 21 demands that only one recipe (campaign) must be selected during one time period.

$$1 = \sum_{\{l,p,r\} \in R^P} \alpha_{lprt}^{rec} \quad \forall \{l,p\} \in P^L, t \in T \tag{21}$$

Equation 22 determines the recipes that are used in the first time period.

$$\alpha_{lpr}^{start} \leq \alpha_{lpr1}^{rec} \quad \forall \{l,p,r\} \in R^P, t = 1 \tag{22}$$

Equations 23 to 26 define binary variable β which represents the recipes that are used in at least two consecutive time periods. In the first time period β is equal to zero, as there is no time period before this period. Equations 24 to 26 make the linkage between α and β. Equations 25 and 26 ensure that β is zero, if α is zero in the same or previous time period.

$$\beta_{lprt}^{proc} = 0 \quad \forall \{l,p,r\} \in R^P,\ t = 1 \tag{23}$$

$$\alpha_{lprt}^{rec} + \alpha_{lprt-1}^{rec} - 1 \leq \beta_{lprt}^{proc} \quad \forall \{l,p,r\} \in R^P,\ t \in T \tag{24}$$

$$\beta_{lprt}^{proc} \leq \alpha_{lprt-1}^{rec} \quad \forall \{l,p,r\} \in R^P,\ t \in T \tag{25}$$

$$\beta_{lprt}^{proc} \leq \alpha_{lprt}^{rec} \quad \forall \{l,p,r\} \in R^P,\ t \in T \tag{26}$$

Production

Processes must be permanently utilized (or idled) during a time period. The available processing hours are equal to the number of hours during a time period minus scheduled maintenance shutdown and lost time during changeovers. As there is no changeover in the first time period, equation 27 only considers shutdown hours. Available processing hours are defined for each process separately so that maintenance hours can be considered for each process. Shutdown hours are defined by the user for any purpose at any time period. They aren't applied regularly.

$$\sum_{\{l,p,r\}\in R^P} h_{lprt}^{rec} = H_{lpt}^{proc} - \varepsilon_{lpt}^{proc} \qquad \forall \ \{l,p\} \in P^L, \ t = 1 \tag{27}$$

$$\sum_{\{l,p,r\}\in R^P} h_{lprt}^{rec} = H_{lpt}^{proc} - \varepsilon_{lpt}^{proc} - \left(1 - \sum_{\{l,p,r\}\in R^P} \beta_{lprt}^{proc}\right) H_{lp}^{changeover} \forall \ \{l,p\} \in P^L, \ t \in T > 1 \tag{28}$$

Each recipe has minimum and maximum throughput boundaries (tons/hour).

$$h_{lprt}^{rec} \underline{Q}_{lpr}^{proc} \le y_{lprt}^{rec-tot} \le h_{lprt}^{rec} \overline{Q}_{lpr}^{proc} \qquad \forall \{l,p,r\} \in R^P, t \in T \tag{29}$$

Production hours are bounded between minimum campaign length and available processing hours including shutdown hours.

$$\alpha_{lprt}^{rec} H_{lpr}^{camp} \le h_{prt}^{rec} \qquad \forall \ l \in L^{mill}, p \in P_l^{mill}, r \in R_p^{proc}, t \in T \tag{30}$$

$$h_{lprt}^{rec} \le \alpha_{lprt}^{rec} (H_{lpt}^{proc} - \varepsilon_{lpt}^{proc}) \qquad \forall \ l \in L^{mill}, p \in P_l^{mill}, r \in R_p^{proc}, t \in T \tag{31}$$

Equations 32 to 34 are related to the mass balance. Equation 32 links the material conversion from feedstock to products. Linear recipe functions are used to represent process where raw material consumption depends on the utilization rate of the equipment employed. Equation 33 relates the material output to the total output of a process, while equation 34 aggregates the total output of a material during one time period.

$$x_{lmpt}^{proc} = \sum_{\{l,p,r,m\}\in M^{R-in}} a_{lprm}^{input} y_{lprt}^{rec-tot} \qquad \forall \{l,p,m\} \in M^{P-in}, t \in T \tag{32}$$

$$y_{lprmt}^{rec} = a_{lprm}^{output} y_{lprt}^{rec-tot} \qquad \forall \{l,p,r\} \in R^P, \{l,p,r,m\} \in M^{R-out}, t \in T \tag{33}$$

$$y_{lmpt}^{proc} = \sum_{\{l,p,r,m\}\in M^{R-out}} y_{lprmt}^{rec} \qquad \forall \{l,p,m\} \in M^{P-out}, t \in T \tag{34}$$

Processes require or produce steam and/or electricity for their operation. Equations 35 to 38 calculate the steam and electricity production/consumption of processes based on the recipe used.

$$v_{lpt}^{output} = \sum_{\{l,p,r\}\in R^P} b_{lpr}^{output-steam} y_{lprt}^{rec-tot} \qquad \forall \ \{l,p\} \in P^L, t \in T \tag{35}$$

$$v_{lpt}^{input} = \sum_{\{l,p,r\}\in R^P} b_{lpr}^{input-steam} y_{lprt}^{rec-tot} \qquad \forall \ \{l,p\} \in P^L, t \in T \tag{36}$$

$$w_{lpt}^{output} = \sum_{\{l,p,r\}\in R^P} b_{lpr}^{output-elect} v_{lpt}^{output} \qquad \forall\ \{l,p\} \in P^L, t \in T \tag{37}$$

$$w_{lpt}^{input} = \sum_{\{l,p,r\}\in R^P} b_{lpr}^{input-elect} y_{lprt}^{rec-tot} \qquad \forall\ \{l,p\} \in P^L, t \in T \tag{38}$$

The steam balance must be satisfied. Enough steam must be produced by boilers and other steam producing equipments to satisfy the needs of other steam consuming processes. However, extra steam may be produced and vented off if not necessary, as represented in equation 39.

$$\sum_{\{l,p,r\}\in R^P} (v_{lpt}^{output} - v_{lpt}^{input}) \geq 0 \qquad \forall\ \{l,p\} \in P^L, t \in T \tag{39}$$

Before presenting the rest of the project methodology, the case study is introduced in the next section. The case study is used to concretize the methodology.

2.4 Case study introduction

In the FBR context, there are two major classes of products that can be produced: large-scale commodity products, and low-volume/high-value fine/specialty products. The commodity chemicals are mainly limited to biofuels, e.g. ethanol, butanol, diesel. The idea that supports the production of these products is that there is a huge market for such commodities in the fuel market, especially in the United States. In contrast, fine and specialty chemicals are said to be promising elements of an FBR product portfolio because they have bigger margins compared to P&P products, and also better market with less competition, so that the FBR does not have to compete with huge well-established commodity petrochemical products. Because fine and specialty products are produced in smaller volumes, they need less feedstock. This is a competitive advantage, because biomass procurement is a great challenge.

An analysis of biorefineries conducted by the National Renewable Energy Laboratory (NREL) (Lynd, Wyman, C., Laser, M., Johnson, D., & Landucci, 2002) addressed the importance of coproducing high-value low-volume products along with a primary product. According to this report, the advantages of such a product portfolio compared to dedicated production of a single commodity product can be classified into two levels: long-term and short-term. The long-term advantages are summarized as follows:

- Product diversity mitigates risks associated with seasonal demand cycles and market downturns.

- If selected coproducts have the potential to become platform intermediates in future, their commoditization will be fostered by taking advantage of the economies of scale provided by producing small amounts of the coproduct in a commodity-producing biorefinery. An ethanol plant producing succinic acid, lactic acid, and/or butanol as coproducts is an example. As mentioned in the NREL report, early-generation ethanol biorefineries can serve as incubators for chemicals that can then become high-volume products in their own right.

The short-term advantages are as follows:

- Revenues from high-value coproducts reduce the selling price of the primary product.
- The economies of scale provided by a full-size biomass refinery lower the processing costs of low-volume/high-value coproducts.
- Biomass refineries maximize the value generated from heterogeneous feedstock, making use of component fractions.
- Common process elements are involved in producing fermentable carbohydrates, regardless of whether one or more products are produced.
- Coproduction can provide process integration benefits (e.g., meeting process energy requirements with electricity and steam cogenerated from process residues).

Given that, two major strategies with regard to the products that can be produced in an FBR have been proposed: production of large-volume/low-value commodity products along with low-volume/high-value products, and production of specialty chemicals (Yun, Kim, Pak, & Park, 2009; Luo, Voet, Huppes, 2010). The characteristics of two strategies are compared in Table 2-1.

Table 2-1 Characteristics of biorefinery product strategies

1st strategy: Commodities + Specialties	2nd strategy: Specialties
Large market	Small market
Mature technologies	Immature technologies in general
Competitive market	Lower competition in the market
Needs large amount of feedstock	Needs small amount of feedstock
Low margin/high price volatility	High margin/low price volatility

In this work, two product portfolio options are defined considering the two abovementioned product strategies. The biorefinery strategy to be pursued for both portfolio options is the adjacent or decoupled biorefinery, i.e. the new biorefinery processes will not be tightly integrated with the existing mill. Both options and their related strategies were defined via discussion with one of the industrial partners of this research.

The first portfolio option, representing the first strategy, includes the production of Fischer-Tropsch liquids (FTL) and jet fuel (JF). FTL comprise of light fraction (LFTL) which is naphtha, medium fraction (MFTL) which is diesel, and heavy fraction (HFTL) which is wax. In this portfolio, the diesel is a commodity, whereas wax and JF can be interpreted as value-added products. As the biorefinery pathway taken for this portfolio is thermochemical, this portfolio is called *Thermochemical option*. Thermochemical option was defined based on a real case study.

The second portfolio option, representing the second strategy, involves the production of a set of value-added organic acids, including lactic acid (LA), succinic acid (SA) and malic acid (MA). LA and MA are the products with the lowest and highest prices, respectively. The biorefinery pathway related to this option is biochemical. Therefore, this portfolio option is called *Biochemical option*. This option is hypothetical and defined to show the value of value-added chemicals and to compare them with commodities. LA is the most known product among these three acids and can be used to make plastics, fibers, solvents and oxygenated chemicals. Besides, LA is a relatively mature fine chemical to which new applications are found every year. By 2015, its global market will reach 329,000 tons a year (Datta & Henry, 2006). MA is a very high value chemical that has usages in food and pharmaceutical industries. But SA has got the most attention over the past years among these acids. It currently provides the basic four-carbon backbone for a wide range of products including pharmaceuticals, coatings, polymers and resins. The current market of 30,000 tonnes will expand six-fold by 2015 due to introduction of bio-succinic acid. What gives a competitive advantage to SA is its low production cost in biochemical pathways compared to its oil-based counterpart.

2.4.1 Thermochemical option

The whole idea of the thermochemical option is to gasify biomass into synthesis gas (syngas), which contains the desired hydrogen and carbon monoxide, with some methane and other hydrocarbons. The syngas either can be used to produce biofuels that can be further blended into typical gasoline or naphtha pools to supply fuel gas to processes and systems where gaseous fuels are more appropriate then solid fuels, or it can be used for production of biochemicals. In this thesis, production of liquid fuels was chosen.

2.4.1.1 Summary

This system is designed to produce 8.2 million gallons per year of clean renewable FTL. The FTL beak-down is 1300 gallons/day of LFTL, 11500 gallons/day of MFTL (diesel) and 10500 gallons/day of HFTL (wax). Diesel can be converted to JF. The feedstock is 500 bone-dry tons per day of woody biomass comprised of unmerchantable wood chips, forest residues, sawmill residues and hog fuel. The project is based on two technology modules; the reforming and gasification process, and the generic Gas-to-Liquid (GTL) process, using Fischer-Tropsch process. Gasification is the sub-stoichiometric oxidation of a biomass to produce a gaseous mixture containing carbon monoxide, carbon dioxide, methane, hydrogen, hydrogen sulfide and other hydrocarbons. Steam reformation is a more specific chemical reaction whereby steam reacts with organic carbon to yield carbon monoxide and hydrogen. The Fischer-Tropsch catalyst based GTL process converts the syngas into various multi-carbon fraction liquid hydrocarbon fuels. The study basis for the Fischer-Tropsch unit operations is a generic fixed bed catalyst system.

2.4.1.2 Process description

The processing steps include:

- Biomass receiving and wet storage
- Biomass dryer and dry storage
- Reformer/gasifier
- Gas-to-liquids conversion
- Product separation and storage
- Hydro-treating process

Biomass drying and heating and pyrolysis occurs within the steam reformer. The pyrolysis releases volatile components in the form of methane, hydrogen, carbon monoxide, carbon dioxide, and other hydrocarbons, then char reforming and partial oxidation occurs, creating a medium Btu hydrogen rich syngas that can be used to offset fossil fuels, generate clean power or produce biofuels and biochemicals. In this thesis, it is assumed that the syngas is cleaned, compressed, and processed in a typical Fischer-Tropsch reactor to produce liquid fuels. Fixed bed Fischer-Tropsch GTL processing is a mature technology. The syngas generated in the steam reformer is first cooled in a heat recovery steam generator (HRSG), where the heat is recovered in the form of high pressure steam. The cooled syngas then goes through a cold syngas clean-up train comprised of a venturi scrubber to remove any particulate carry-over, a gas cooler to condense remaining steam, then an H_2S scrubber to remove H_2S. The clean syngas after compression passes through an ammonia scrubber and sulfur guards to remove residual ammonia and H_2S that could poison the catalyst in the gas-to-liquids reactor. The product stream from the reactor is separated in three different cuts according to their boiling point. A hydro-treating process can be used to convert diesel to JF. The liquid fuel streams produced can be used in a conventional refinery. A fourth stream is tail gas which is distributed to the lime kiln, the duct burner, and the PC heaters, providing the indirect bed heating for the volatilizing of the biomass and the endothermic steam reforming reaction. A simple block flow diagram of this process is shown in Figure 2-3.

There is an inherent flexibility on the process with regards to the percentage of the FTL fractions that can be produced by the GTL process. The nominal operating point yields 55% diesel and 45% wax. This percentage can change to 45% diesel and 55% wax. In order to model this behaviour in the SC mathematical formulation, three recipes representing three operating modes have been defined. First recipe yields 55% diesel and 45% wax, second recipe yields 50% diesel and 50% wax, and third recipe yields 45% diesel and 55% wax. Each recipe has an associated production cost. Changing from one recipe to another recipe incurs changeover time and changeover cost which are considered in the SC mathematical formulation.

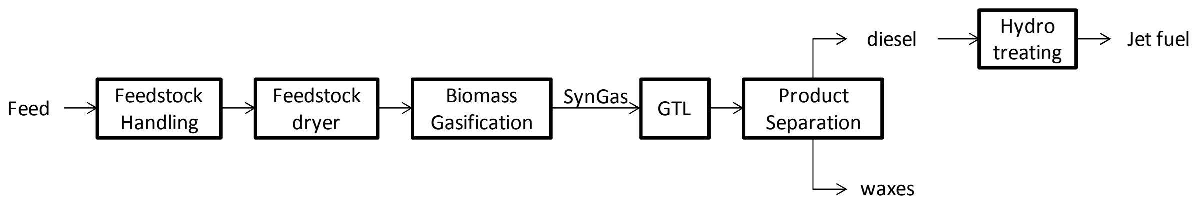


Figure 2-3 Thermochemical option: Block flow diagram

2.4.1.3 Process data

The process data are presented in Table 2-2. Data include product and feedstock prices, utility costs, transportation, storage and sales costs for each product, as well as production cost for each recipe and the capital cost. All data have been provided by the industrial partner.

Table 2-2 Process data for Thermochemical option

Item price	Unit	Value	Description
Product			
Naphtha	$/Gal	2.05	Base case product price
Diesel	$/Gal	3.07	
Wax	$/Gal	5.12	
Jet fuel	$/Gal	4.05	
Feedstock			
Wood chips	$/Wet ton	35.84	Base case biomass price Transportation cost is included
Forest residues	$/Wet ton	35.84	
Sawmill residues	$/Wet ton	35.84	
Hog fuel	$/Wet ton	35.84	
Utility			
Natural Gas	$/MMBTU	8	Base case price
Electricity	$/MWh	64	
Water	$/KGal	0.5	
Boiler Feed water	$/KGal	1	
Waste water treatment	$/KGal	1.3	
Product transportation			
Naphtha	$/Gal	0.15	
Diesel	$/Gal	0.05	
Wax	$/Gal	0.15	
Jet fuel	$/Gal	0.05	
Storage cost	%	10	Storage cost for all materials is 10% of material price
Sales cost			
Naphtha	%	1	Sales cost for all products is equal to a percentage of product price
Diesel	%	1.66	
Wax	%	1	
Jet fuel	%	1.66	
Production cost			
1st recipe	$/Gal	1.1	Base case cost
2nd recipe	$/Gal	1.5	
3rd recipe	$/Gal	1.9	
Jet Fuel	$/Gal	1.4	
Capital cost			
FTL production	$MM	112.5	$51 MM grant
Jet Fuel production	$MM	26	

2.4.2 Biochemical option

In the biochemical option, the biomass goes through a series of biochemical treatments to be converted to organic acids. After pre-treatment steps and separating cellulose from other wood components, enzymatic hydrolysis of cellulose and fermentation of the resulting glucose is used for acid production. The process design also includes feedstock handling and storage, product purification, wastewater treatment, lignin combustion, product storage, and required utilities.

2.4.2.1 Summary

The system consists of two lines in parallel. The first line produces 150 tons/day of LA. The second line is flexible and can produce 200 tons/day of SA in one production mode and 200 tons/day of MA in another production mode. Both lines need 1000 bone-dry tons per day of woody biomass in aggregate. Woody biomass is pre-treated and extracted to its three major components. Cellulose is converted to glucose and then fermented to acid. It was assumed that the extracted hemicellulose, which is in the form of xylose, can be converted to xylitol. Lignin can also be combusted to produce energy. The remaining of required energy is produced by fuel.

2.4.2.2 Process description

The block flow diagram of the process is shown in Figure 2-4. The processing steps involve:

- Feedstock handling and storage
- Pressurized low polarity water (PLPW) extraction
- Enzymatic hydrolysis
- Fermentation; glucose to acids and xylose to xylitol
- Boilers and Recovery systems, including salt recovery, acidification, neutralization, acid recovery, ion exchange purification

As illustrated in Figure 2-4, all processing steps in both lines are similar up to the recovery systems. The PLPW extraction process extracts the major components of the wood. The hemicellulose fraction mainly containing xylose and other C5 sugars is sent to the fermentation process to be converted to xylitol. The stream containing cellulose and lignin is sent to the enzymatic hydrolysis step, in which cellulose is converted to glucose and lignin remains unchanged. Up to this point, all processing steps and their outputs are similar in both lines. From this point onwards, glucose goes through a fermentation process, which is an identical unit operation on both lines, however, different products (LA, SA, MA) can be obtained in each line according to the microorganism used.

In the first line, glucose is fermented and converted to LA. Excess calcium hydroxide/carbonate is added to the fermenters to neutralize the acid, and to produce a calcium salt of the acid in the broth. The calcium lactate-containing broth is filtered to remove cells, carbon treated, evaporated and acidified with sulfuric acid to convert the salt into lactic acid and insoluble calcium sulfate, which is removed by filtration. The filtrate can be further purified using carbon columns and ion exchange and evaporated to produce technical grade lactic acid. For the high-purity product, the technical-grade lactic acid is esterified with methanol or ethanol, and the ester is recovered by distillation, hydrolyzed with water, evaporated and the alcohol recycled. This separation process yields a pure product (Datta & Henry, 2006).

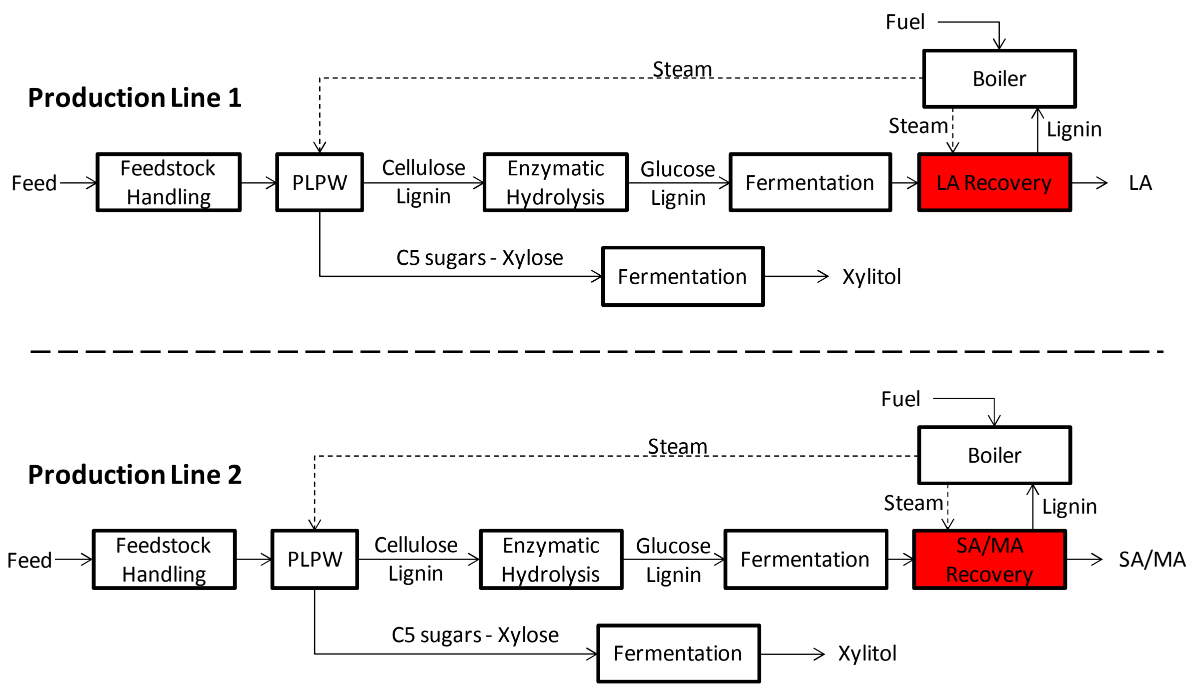


Figure 2-4 Biochemical option: Block flow diagram

In the second line, glucose is diluted with process water and is sterilized in a steam injection sterilizer. Required nutrients and salts are continuously combined with the glucose prior to its addition to the fermenter. Calcium hydroxide slurry is added to the fermenters to neutralize the fermenter broth and to precipitate the succinate as calcium succinate. The calcium succinate is recovered from the fermenter broth by first concentrating the slurry using hydrocyclones, then pressing the slurry in two belt press filters in series. The cake from the filter is washed and the slurry is acidified, using sulfuric acid, to convert the calcium succinate to SA and insoluble calcium sulfate (gypsum), which precipitates. The SA/calcium sulfate slurry is neutralized in a subsequent vessel using sodium hydroxide as the base. The calcium sulfate is recovered in belt press filters and then is fed to a screw press to remove most of the water. The filtrate from the belt press filters containing the SA is sent through a series of ion exchangers. The highly purified SA is concentrated in a multi-effect evaporator (Bozell & Landucci, 1993).

2.4.2.3 Process data

The process data are presented in Table 2-3. Feedstock is similar to what presented in Table 2-2.

Table 2-3 Process data for Biochemical option

Item price	Unit	Value	Description
Product			
Lactic acid	$/Ton	850	Base case product price
Succinic acid	$/Ton	1000	
Malic acid	$/Ton	1800	
Xylitol	$/Ton	1000	
Utility			
Natural Gas	$/MMBTU	8	Base case price
Electricity	$/MWh	64	
Water	$/KGal	0.5	
Boiler Feed water	$/KGal	1	
Waste water treatment	$/KGal	1.3	
Product transportation			
Lactic acid	$/Ton	33	
Succinic acid	$/Ton	25.5	
Malic acid	$/Ton	25	
Xylitol	$/Ton	35	
Storage cost	%	10	10% of material price
Sales cost			
Lactic acid	%	2	Sales cost for all products is equal to a percentage of product price
Succinic acid	%	2	
Malic acid	%	2	
Xylitol	%	2	
Production cost			
Lactic acid	$/Ton	300	Base case cost
Succinic acid	$/Ton	320	
Malic acid	$/Ton	370	
Xylitol	$/Ton	50	
Capital cost			
Whole system	$MM	122	

2.5 Overall methodology

In the strategic design of an SC, long-term decisions should be made. Such decisions include the type of products that should be produced, the technologies that can be used, the number, location and capacity of each type of facility, and the target markets. In a practical problem, it is difficult to address all these decision within a single SC optimization framework. Instead, it is preferable to pursue a hierarchical methodology that addresses all these factors in a stepwise manner.

Because of the combinatorial aspect of such design problems, the hierarchical methodology might miss the global optimum. This is due to the fact that all possible options at each step or their interaction with each other might be missed. However, this methodology does not seek to identify a global optimum. Rather, it seeks a set of feasible and practical biorefinery options (near-optimal solutions) that a company can strategically pursue. The decision as to what biorefinery strategy to take depends on many factors, most of which cannot be reflected in an optimization problem, e.g., understanding the market and market strategies, emerging products and technologies, the capabilities of existing SC assets, and potential partners. Many of these aspects can be addressed in different scenarios instead of being modeled into an optimization formulation. In this way, a simpler model will be solved, with more practical results.

Companies seek a set of biorefinery options that would significantly improve their business model. This should include the optimum and near-optimum solutions. This set of possible strategies should be pursued by a company in parallel with potential partners to establish mutual interests and to address most effectively the competitive disadvantages of forestry companies, such as lack of capital. This methodology would end up with a set of solutions. An MCDM framework can be used to find the best option from a specific company's point of view, considering all the complexities involved in the industrial arena.

To achieve a stepwise methodology, some of these decisions must be made by integration with other methodologies. This idea was proposed by Mansoornejad, Chambost, and Stuart (2010), as can be seen in Figure 2-5. The set of products that should be produced can be determined by a product portfolio definition methodology (Chambost & Stuart, 2007). Then, technologies that can be used are chosen through a techno-economic study (Hytonen, 2011). The result will be a set of product/process portfolios which were screened out from the non-profitable ones based on a preliminary market/techno-economic study. From this point, two separate analysis tools, one related to SC and one related to LCA, are utilized to analyze the remaining portfolios from different perspectives. Each of these analyses, along with product portfolio definition and techno-economic study, provide several metrics that can ultimately be used in an MCDM. An MCDM considers several criteria provided from different analysis tools and helps making decision by taking into account different perspectives.

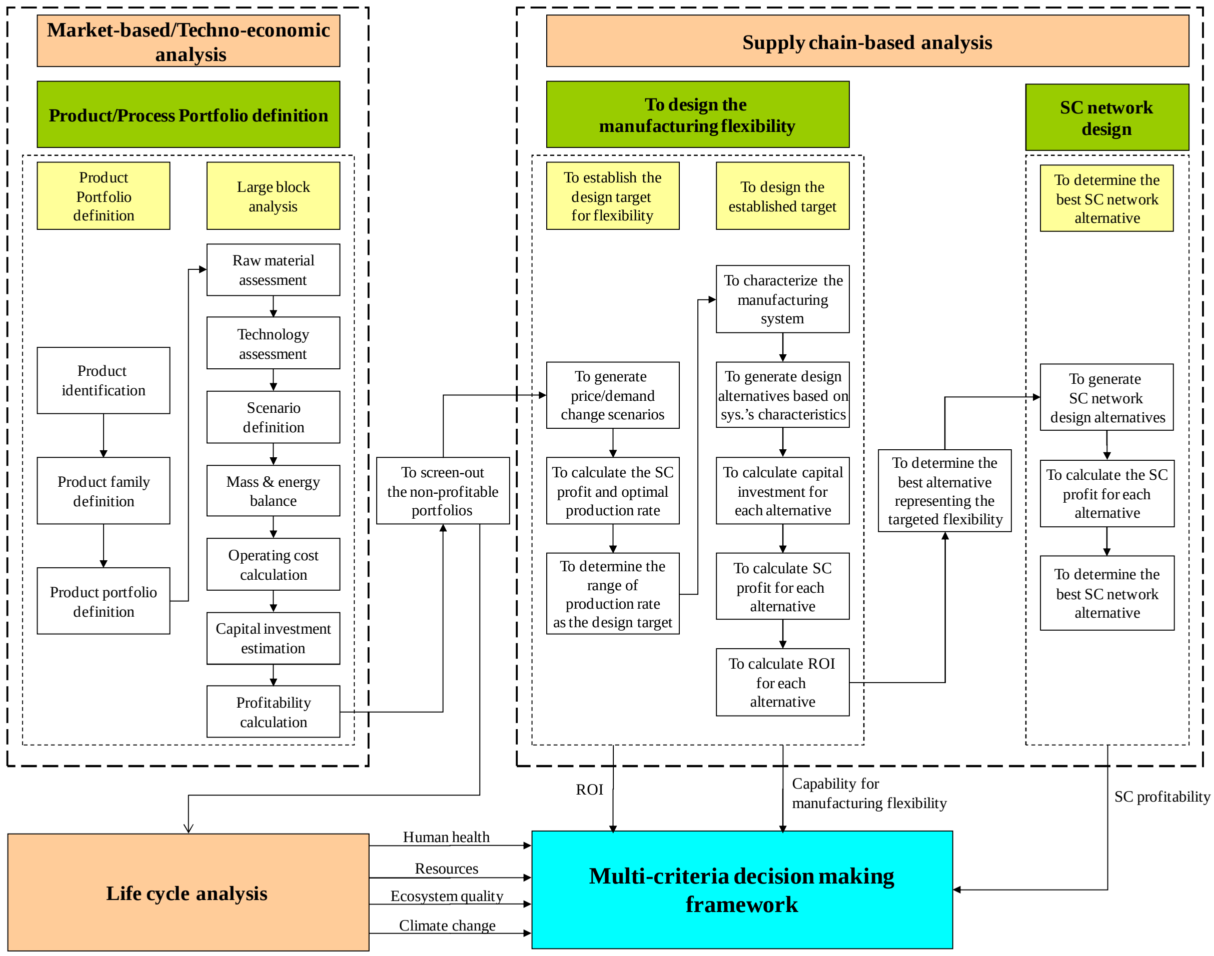


Figure 2-5 Stepwise methodology for FBR decision making (Mansoornejad et al., 2010)

This thesis focuses on the SC-related part of this stepwise methodology, i.e. the SC-based analysis. The methodology related to this part has been evolved since it was first presented Mansoorneja, Chambost, and Stuart (2010). However, the main philosophy behind those first thoughts is still valid. As can be observed in Figure 2-5, the SC-based analysis has two major parts; designing the manufacturing flexibility and designing the SC network. Similarly, the aspects that are addressed by the hierarchical methodology presented in this thesis include:

1. Targeting the design of flexibility, including the determination of the production capacity as well as the operating window as a design target, i.e., range of production rates for each process, showing the flexibility capability of the plant.
2. SC network design, including determination of the number of facilities of each type, the location of each facility, and the capacity of warehouses and distribution centers, as well as partner selection. Note that network design-related decisions are made through the generation of alternatives. These alternatives must be generated based on practical aspects of the problem that can be addressed via discussion with company board of executives considering all features of the existing SC.

What has been added to methodology is the evaluation of the phased implementation approach, including the analysis of the implementation strategies for each biorefinery option and comparing the results, and the evolution of the methodological steps. The hierarchical methodology for SC strategic design is illustrated in Figure 2-6.

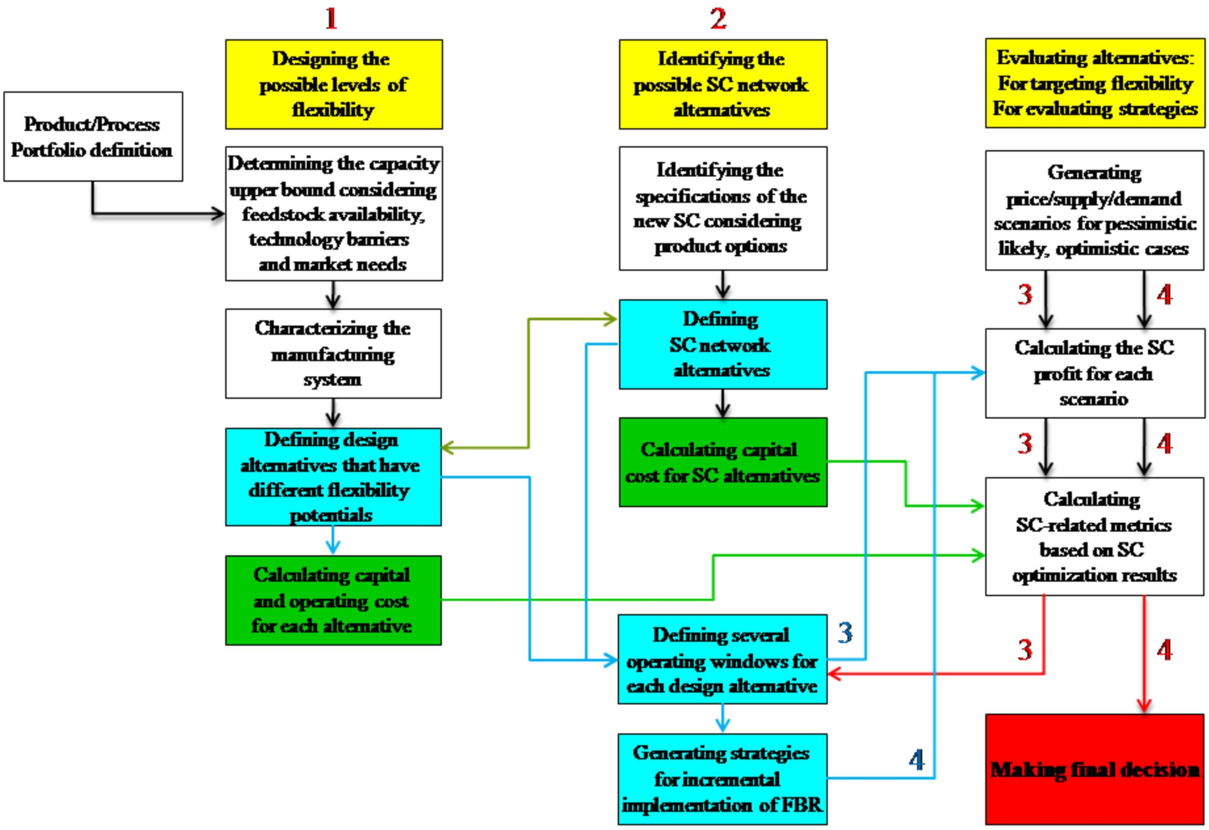


Figure 2-6 Hierarchical methodology for SC strategic design

The overall goal of this thesis is to show how a SC-based methodology can enable decision-makers to 1) define various biorefinery options systematically by targeting their process flexibility and designing their SC network, 2) analyze their operational performance from an SC perspective in different market scenarios, and 3) evaluate their implementation strategy under different market conditions based on the effects of the design of each option on its tactical-operational performance.

The hierarchical methodology consists of four main parts:

1. Process design: Designing possible levels of flexibility (process alternatives)
2. SC network design: Designing possible SC networks (SC network alternatives)
3. Targeting the level of flexibility for each alternative using SC optimization
4. Generating implementation strategies based on defined process/SC network alternatives and evaluating them for making the final decision

In this methodology, first, process design alternatives representing different potentials of flexibility are defined. In the second part, SC network alternatives are defined based on the assets of the existing SC and resources that are needed for new products. Then the process and the SC network alternatives are combined to create a set of process-SC network alternatives, called combined alternatives. In the third part, the SC model is run for different levels of volume flexibility of each combined alternative, in case of several market scenarios. The SC profit of each combined alternative is calculated at the operational level over a year, and by considering profit and capital costs, profitability associated with each level of flexibility of each alternative is estimated. Additionally, the robustness of each alternative against all market scenarios is determined using a relevant metric, which is presented further in detail in the synthesis section (Section 3). The level of flexibility of the alternative that has the best performance is set as the targeted level of flexibility. In the fourth part, several implementation strategies are defined based on the targeted level of flexibility. The advantages and constraints of the mill must be considered when defining strategies through discussions involving the executive board of the mill. SC model is run for each strategy in case of several market scenarios and the performance of each strategy at the operational level is evaluated. Performance metrics, i.e. profitability, robustness and flexibility, are used to evaluate the performance of the alternatives.

2.5.1 Boundaries of the methodology and the SC formulation

In this part, the boundaries of the methodology and the SC formulation, i.e. what is given by other methodologies or is defined, what is wanted, what is defined or determined by the methodology and the SC formulation, and what is not in the scope of this work and is not calculated by the SC formulation, are explained.

- **Given**
  - A set of options including product portfolios and their associated process alternatives
  - Current conditions of the mill that restrict the choice of SC network alternatives and implementation strategies
  - A finite set of market scenarios representing market volatility
- **Wanted**
  - Biorefinery options with targeted level of flexibility and designed SC network
  - The implementation strategy of each biorefinery option
- **Defined by the methodology**
  - Process alternatives with different potentials for flexibility (defined by engineering heuristics)
  - SC network alternatives (considering process alternatives and mill conditions)
  - The implementation strategy of each biorefinery option (considering process/SC alternatives and mill conditions)
- **Calculated by the SC model**
  - SC metrics (SC profit and profitability, flexibility, robustness)
- **Not directly calculated by the SC model**
  - Design decisions (capacity and flexibility of processes, SC network configuration)

Design variables are defined deterministically in each alternative and, for deterministic alternatives, the SC model calculates all SC metrics. Metrics determine which alternative is the best. Thus, the SC model makes design decisions implicitly. Table 2-4 summarizes the boundaries.

Table 2-4 Boundaries of methodology and SC formulation

Item	Input from other methodologies	Defined/Calculated by the methodology	Calculated by the SC model
Biorefinery options - Product portfolios - Process alternatives	 ✓ ✓		
Level of flexibility of each process alternative		✓	
SC network alternatives		✓	
Implementation strategies		✓	
SC metrics - Profit and profitability - Flexibility - Robustness			 ✓ ✓ ✓

In the next parts of this section, the methodology is presented in details.

2.5.2 Process design

In the first part of the methodology, i.e., process design, there are four steps: determining the upper bound for production capacity, characterizing the manufacturing system in terms of product and volume flexibility to identify the modifications needed for the processes to become more flexible, generating design alternatives with different flexibility potentials, and calculating capital and operating cost for each design alternative.

2.5.2.1 Determining the capacity upper bound

The maximum possible capacities for each process are identified by considering three major factors: market demand, feedstock availability, and technical barriers. In the case of biorefinery implementation, feedstock availability is the most important factor in calculating the capacity upper bound. The availability of feedstock from different sources in and around the mill region is studied, and the cost of bringing the feedstock to the mill is estimated. Various factors should be considered in calculating the amount of available feedstock, e.g., price, proximity, seasonality, and transportation. A market analysis is carried out to determine the market size and market share of the targeted products based on the available amount of feedstock. Finally, considering the available technologies and the possible production rates from a technical point of view as provided by the technology providers, maximum capacity is identified.

2.5.2.2 Characterizing the manufacturing system

Every process is designed in a way that can operate feasibly under changing conditions and over a range of production rates. The methodology presented in this work focuses on the volume-flexibility design for an FBR to enable it to be profitable under volatile market conditions. Note that the methodology does not deal with early-stage design, rather considers the existing processes with their inherent flexibility and will retrofit the design in case the inherent flexibility is not sufficient to handle market volatility.

To design a flexible production system, this system must be characterized based on the following aspects:

- Process configuration: It should be verified whether the products can be produced in series, i.e., they are in one product family (Figure 2-7.a), or whether they should be produced in parallel lines, because they are not from one family (Figure 2-7.b).
- Product flexibility: It should be verified whether the system is a dedicated one in terms of products (Figure 2-7.a and Figure 2-7.b), or whether several products can be produced in a single line in different production modes (Figure 2-8).
- Volume flexibility: It should be verified whether the process can handle a range of production rates and whether the inherent flexibility of the process is enough or not.

2.5.2.3 Defining design alternatives with different flexibility potentials

The goal of this step is to define several *process alternatives*, each representing a potential of flexibility. This task is very much case-dependent. Based on the characterization of the manufacturing system, different strategies can be used to increase the flexibility.

Chemical processes are designed to operate at maximum capacity, which is generally called nominal production rate. Under changing conditions the operating rate must change to some extent. The distance (as a percentage of nominal rate) between the lowest point below the nominal production rate at which the process can operate, and the designed nominal production rate is called the turndown ratio. All chemical processes have an inherent turndown ratio. But sometimes it is desirable to have a greater turndown ratio than the inherent one. A simple way is to divide the production line, or the part of it that limits the process, into smaller lines, so that if the production rate must be decreased, some of these smaller lines can be shut down.

A similar strategy that can be used to make a system more flexible is to add extra equipment or process sections and keep them on standby. This strategy will work for increasing capacity. The number of equipment that restricts the process can be increased so that when production increases, more capacity can be provided by the standby equipment.

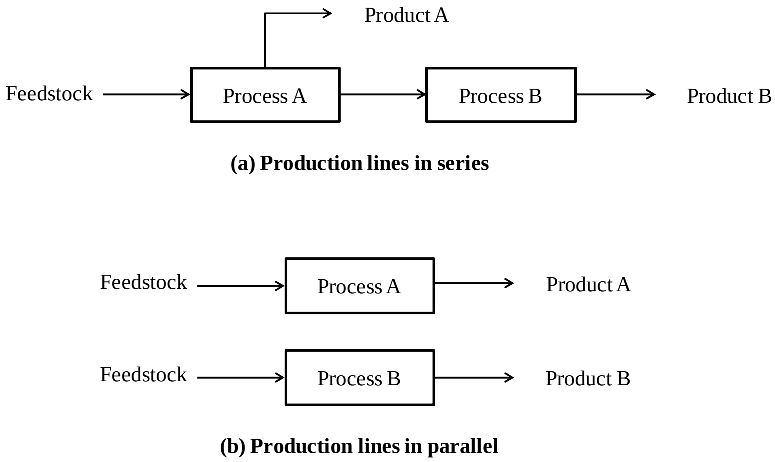


Figure 2-7 Separate production lines: (a) in series, (b) in parallel

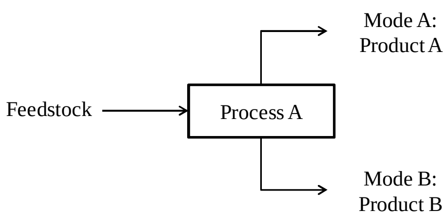


Figure 2-8 Flexible production line

2.5.2.4 Calculating capital and operating costs for each design alternative

Finally, the required capital investment for each design alternative and the operating cost associated with the nominal production rates are calculated. These costs will be used to estimate the profitability of each design alternative under different market scenarios.

Up to this step, a few number of design alternatives with different potentials of flexibility have been defined. However, the flexibility of each process has not been targeted yet. As the goal is to target the design of flexibility using SC optimization, in the next part the SC network alternatives must be defined and combined with design alternatives. Then, the SC model can be used to target the flexibility of each process.

2.5.3 SC design

In the strategic design of the SC network, decisions are made to redesign an already established SC network with all its existing assets. The SC of a forestry company should be redesigned so that it can be used in the FBR. In this methodology, the SC network design is performed in two steps. First, the specifications of the new SC are identified based on the characteristics of the new product options. Then SC network alternatives are defined. These SC network alternatives are combined with the process design alternatives defined in the previous part of the methodology, and in the next part, SC optimization is used to calculate the SC profitability of each alternative. Interaction between this part and the previous part is necessary.

2.5.3.1 Identifying the specifications of the new SC with product options

The SC networks of forest-products companies are in place with their own existing assets. Depending on the processes used in the mills, different facilities exist on the site. However, some processing steps are common among all processes in the mill, and therefore similar facilities and assets can be used or redesigned to be able to handle larger volumes.

Biomass receiving, processing, and storage areas in the mills generally include a biomass receiving and unloading station, biomass storage with a reclaimer, biomass processing involving a biomass size-reduction process, cleaning and wet storage, and finally, biomass drying and dry storage. These facilities are used regardless of the fate of the biomass, i.e., the final product. Therefore, the design process should identify whether the new processes need the same facilities and whether the existing facilities have enough capacity for the larger amount of biomass that will be brought to the mill. If new or additional facilities are required, there is a need to investigate how those facilities should be modified or be added to the site to enable the mill to accept more biomass. Moreover, existing boilers, turbines, and wastewater treatment plants can be used by the new processes, which will significantly reduce the required capital cost for implementing the FBR.

On the product side, the characteristics of new products must be taken into account to redesign the SC network. Each product has specific properties and characteristics which imply specific facilities for transportation and storage. Some products can be stored in warehouses, while others must be stored in tanks. Moreover, some products are transferred by truck or train, while others should be transported in a tanker or by pipeline. Therefore, the specifications of each product must be identified so that they can be addressed when defining SC network alternatives.

2.5.3.2 Defining SC network alternatives

With the existing SC assets and the characteristics of the products, the specifications of the new SC network can be identified. Based on these specifications, several *SC network alternatives* can be defined, which reflect the needs of the new SC network as well as the policies and restrictions of the company. Several issues should be addressed when generating these alternatives;

- Partnership: Collaborating with other companies whose expertise brings value to the company's business model must be considered in the SC network design. Partners can cooperate in producing a product, delivering the product, buying the product, and/or selling the product to the market. In this way, a part of the partner's SC assets will be used, and less capital will be needed for establishing the new SC network.
- Location and capacity of distribution centers: Based on the location of the plant, several target markets might exist in the areas around the plant. Therefore, different distribution centers with different capacities can be assigned to the target market areas. The role of partners in this issue is important. They might take the role of seller in the target markets, and they might have the required infrastructure for this purpose.
- Transportation network: Based on the characteristics of the products, different means of transportation can be used for product delivery. Again, partnerships can be used to reduce the capital costs required for establishing a transportation network. Contracts can be made with transportation companies which have a network of trucks or tankers and can simply deliver the products to markets. In addition, partners which buy the products or just deliver them to the market might have their own existing transportation network.

2.5.3.3 Calculating capital cost for SC alternatives

In this step, the capital investment required for redesigning the SC network is calculated. The cost associated with any modification to pre-processing steps, warehousing and transportation system must be addressed.

After defining the SC network alternatives, the process alternatives are assembled to create *combined alternatives*. Each combined alternative involves a process configuration and a SC network related to the products. The capital investment required to redesign the SC network is added to the capital investment needed for the process technologies for each alternative.

2.5.4 Targeting flexibility

The goal of this part is to target the flexibility of each design alternative based on its performance in different market conditions. This part contains three steps: after defining several volume flexibility levels (operating windows) for each design alternative, first, a finite number of market scenarios are generated. Then, for all flexibility levels, the SC profit is calculated for each scenario. Then the profitability of each alternative is estimated for each scenario, and the robustness of each alternative are quantified.

2.5.4.1 Generating market scenarios

To address the uncertainty of market conditions and to reflect market volatility in the decision-making process, a scenario-based approach is used. Each scenario represents a specific market condition with respect to price, supply, and demand. Scenarios are generated in terms of feedstock supply and product demand, as well as feedstock and product prices. Scenarios must be generated to capture different market situations, i.e. pessimistic, likely and optimistic cases should be considered in scenario generation. Another important factor in scenario generation is the time aspect. Scenarios can be generated for different time scales, and depending on the type of decisions to be made in the scenario analysis, scenarios can be generated for the short, medium, or long term. For strategic design-related decisions, scenarios should be generated for the long term, e.g., for a period of several year. As supply, demand, and price change during the year, the values associated with them can vary on a monthly or seasonal basis. Note that buying feedstock and selling products can be done based either on contracts or on the spot market. Contractual prices and demands imply fixed values during specific periods, meaning that the amount of product and its price in the contract can be fixed for the whole period of the contract or can change during certain periods based on the agreements reached at the time of making the contract, while spot prices are generally subject to changes based on the market situation. Therefore, both spot and contractual prices and demands must be addressed in scenario generation. It must be mentioned that scenarios are defined through discussion with the mill's executive board.

2.5.4.2 Calculating the SC Profit for each scenario/operating window of alternative

To target the flexibility of each combined alternative, the profitability of each operating window (level of flexibility) for each combined alternative must be calculated along with other metrics. Therefore, the SC profit associated with each operating window of each alternative in different market situations must first be calculated, and then, using the profit, profitability of each alternative as well as other metrics can be estimated. In this step, the SC profit for each product/process/SC alternative is calculated for every price/supply/demand scenario. To calculate the SC profit, the SC optimization model is used. The model optimizes SC profit by determining which orders to fulfill and calculating the optimum value of production rate related to each product and the flows of material between SC nodes. The overall problem at this stage can be stated as follows.

Given:

- Number and length of time intervals
- Demand and price data for each feedstock, product, market, and time interval for each scenario
- Process configuration based on what was defined in the process design step
- Configuration of the SC network based on what was defined in the SC network design
- Capacity data of the nodes of the SC
- Direct cost parameters, i.e., unit production, transport, handling, and inventory costs based on operating cost calculations;

With the aim of profit maximization, find

- Orders to fulfill: which contracts to make, which spot demand to fulfill
- Production rates of each product for all time intervals and all market scenarios
- Flows of materials between the plants, warehouses, distribution centers, and markets
- SC profit

2.5.4.3 Calculating SC-related metrics based on SC optimization results

To evaluate each product/process/SC alternative, the value of several metrics should be estimated for each alternative. In this thesis, SC profitability, flexibility and robustness are used as SC-related metrics. All these metrics are discussed in detail in the synthesis section. Based on the values of metrics, the best operating window (level of flexibility) for each combined alternative can be identified, and thus, targeted. The metrics are introduced in the next chapter.

2.5.5 Implementation strategy

In this part, considering the defined process/SC network alternatives and the targeted flexibilities as well as the policies and restrictions of the company, several strategies are defined for implementing each alternative. Some alternatives might be implementable in one phase, whereas some other might need more than one phase. Moreover, some alternatives might be the evolution of other alternatives. In this case, the implementation phases of one alternative will be a part of the implementation phases of the other one.

After defining strategies, same steps of part 3 of this methodology, i.e. calculating the SC profit and SC-related metrics, are followed. The values of metrics are used to evaluate each strategy. Furthermore, sensitivity analyses are carried out to identify the most important parameters o which the system and its implementation strategy are most sensitive. Then, Monte Carlo simulation is performed on the identified parameters. The result of Monte Carlo simulation will provide better insight into profitability of each implementation strategy and its robustness against key parameters changes.

CHAPTER 3 PUBLICATION SUMMARY AND SYNTHESIS

3.1 Presentation of publications

The following articles that are published in, or submitted to peer-reviewed scientific journals can be found in Appendices A to E of this thesis.

- Mansoornejad, B., Chambost, V., & Stuart, P. (2010). Integrating product portfolio design and supply chain design for forest biorefinery. *Computers & Chemical Engineering, 34*(9), 1497–1506.
- Mansoornejad, B., Pistikopoulos, E. N., & Stuart, P. (2012). Metrics for Evaluating the Forest Biorefinery Supply Chain Performance. Submitted to *Computers & Chemical Engineering.*
- Mansoornejad, B., Pistikopoulos, E. N., & Stuart, P. (2011). Incorporating flexibility design into supply chain for the forest biorefinery. *The Journal of Science and Technology for Forest Products and Processes, 1*(2), 54-66.
- Mansoornejad, B., Pistikopoulos, E. N., & Stuart, P. (2012). Scenario-Based Strategic Supply Chain Design and Analysis for the Forest Biorefinery. Submitted to *International Journal of Production Economics.*
- Mansoornejad, B., Pistikopoulos, E. N., & Stuart, P. (2012). A systematic biorefinery supply chain design methodology incorporating a value-chain perspective. Submitted to *Pulp and Paper International.*

Other complementary publications listed below are included in Appendices F to J.

- Mansoornejad, B., Chambost, V., & Stuart, P. (2009). Integrating product portfolio design and supply chain design for forest biorefinery. In Proceedings of the *7th International Conference on the Foundations of Computer-Aided Process Design*, Breckenridge, Colorado, US, CRC Press. 1017-1033.
- Mansoornejad, B., Pistikopoulos, E. N., & Stuart, P. (2011). Scenario-Based Strategic Supply Chain Design and Analysis for the Forest Biorefinery. In Proceedings of the *21st European Symposium on Computer Aided Process Engineering*, Chalkidiki, Greece, Elsevier, 1025-1029.

- Chambost, V., Mansoornejad, B., & Stuart, P. (2011). The Role of Supply Chain Analysis in Market- Driven Product Portfolio Selection for the Forest Biorefinery. In Proceedings of the *21st European Symposium on Computer Aided Process Engineering*, Chalkidiki, Greece, Elsevier, 1030-1034.
- Mansoornejad, B. & Stuart, P. Forest Biorefinery Supply Chain Design and Process Flexibility. Book chapter in *Integrated Biorefineries: Design, Analysis, and Optimization*. In Review, M. M. El-Halwagi and P. R. Stuart, Eds.: CRC Press/Taylor & Francis, 2012.
- Mansoornejad, B., Pistikopoulos, E. N., & Stuart, P. (2012). Metrics for Evaluating the Forest Biorefinery Supply Chain Performance. Accepted in *22nd European Symposium on Computer Aided Process Engineering*, London, UK.

3.2 Links between publications

The theoretical background of the methodology was presented in the 7th International Conference on the Foundations of Computer-Aided Process Design in Colorado, US (2009) (Appendix F). This work summarized the generic approach for the SC-based analysis and the way it is used to make a linkage between product/process portfolio definition, targeting the process flexibility and designing the SC network. The paper was chosen as a selected paper and recommended for the FOCAPD special issue of *Computers & Chemical Engineering*, and finally was published in 2010 (Appendix A). The evolution of the methodology, with more details on design heuristics applied for defining the process alternatives, was submitted as a book chapter (Appendix I).

In order to provide required tools for the methodology, the second paper was written on the metrics for evaluating the performance of SC, i.e. quantifying different aspects of an SC performance. Metric of robustness represents the capability of the system in not deviating from the base-case performance in a volatile market. Metric of flexibility quantifies volume flexibility of processes. A conditional-value-at-risk type parameter is also developed to analyze the risk of sales strategies. This paper was accepted for 22nd European Symposium on Computer Aided Process Engineering in London, UK (2012) (Appendix J). The extension of this paper was submitted to *Computers & Chemical Engineering* (Appendix B).

The third paper considers the first half of the methodology regarding targeting the level of flexibility (operating window) using the SC-based analysis. The design methodology, which involves chemical engineering heuristics for process design, is presented. Both case studies were used in this paper to concretize the concept of the work. The paper was published in The Journal of Science and Technology for Forest Products and Processes (2012) (Appendix C).

The second half of the methodology concerning the design of SC through a scenario-based approach was first presented in 21st European Symposium on Computer Aided Process Engineering in Greece (2011) (Appendix G). The extension of this paper was submitted to International Journal of Production Economics (Appendix D). This paper introduces the concept of scenario-based SC design which reflects the practical aspects of designing a SC, such as partnership, via defining SC network alternatives. The scenario-based approach is integrated with SC optimization to identify the best SC network alternatives for a specific company.

The wrap up of the methodology including the phased approach for biorefinery implementation was presented in fifth paper submitted to Pulp and Paper International (Appendix E). The summary of major publications and the linkage between them is illustrated in Figure 3-1.

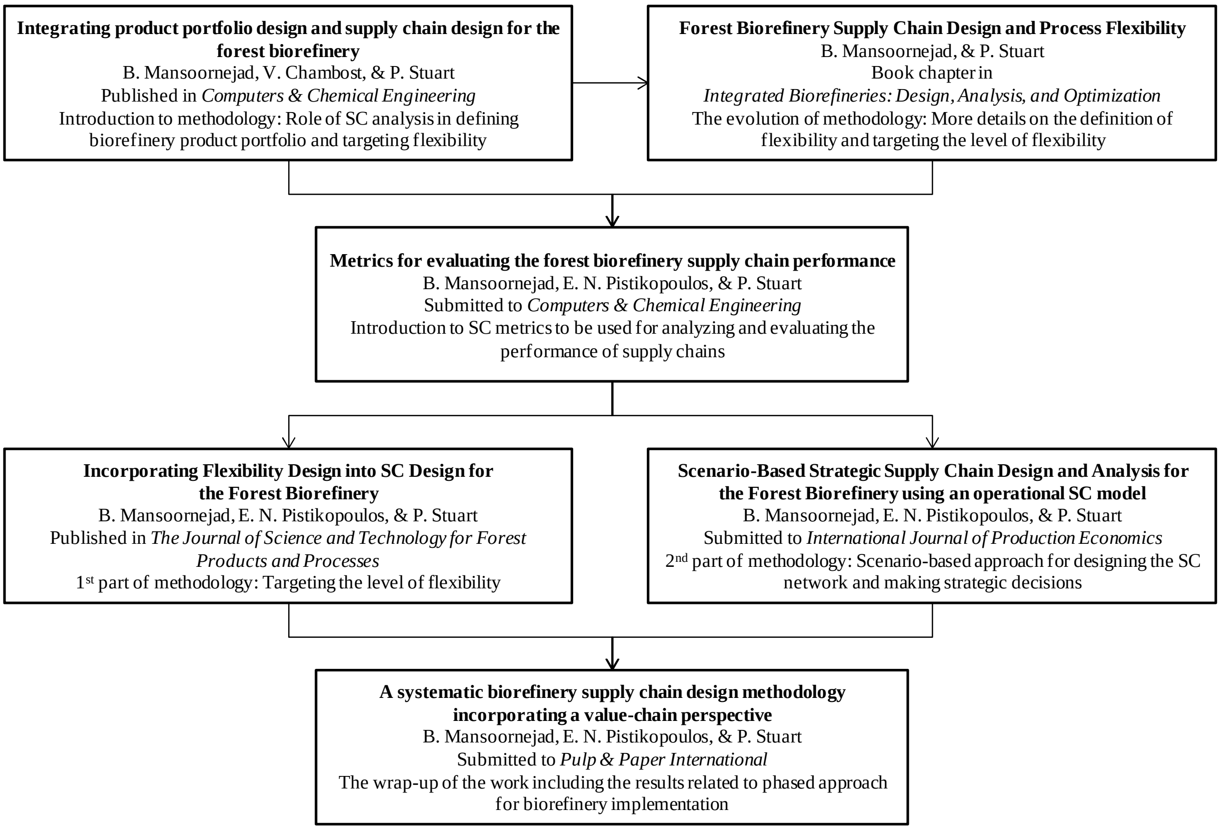


Figure 3-1 Publication summary

3.3 Synthesis

This synthesis presents the main results of the work done in this Ph.D. in order to address the proposed methodology. The focus is on five critical aspects: 1) the importance of margins-based operating policy versus manufacturing-centric approach for improving the profitability of biorefineries, 2) metrics for evaluating the performance of biorefinery SC, 3) targeting the level of flexibility in biorefinery processes through SC-based analysis, 4) designing the SC network through the SC-based approach, and 5) phased approach for implementing biorefineries.

3.3.1 Margins-based policy vs. manufacturing-centric approach

In this section, the result of margins-based policy and manufacturing-centric approach on both biorefinery options, i.e. Thermochemical option and Biochemical option, are analyzed in several market conditions.

3.3.1.1 Thermochemical option

For the Thermochemical option, the SC model is run for the case of FTL production without JF production. The reason is that the goal is to show that by using the inherent flexibility of processes, not by using higher flexibility of a retrofit design, the profitability can be enhanced. The block flow diagram of the Thermochemical option used in this part of the study is shown in Figure 3-2.

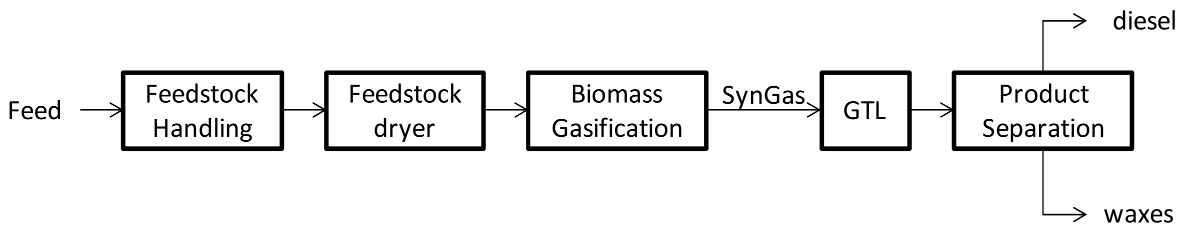


Figure 3-2 Block flow diagram: Thermochemical option

In order to analyze the performance of this option in different market conditions, five market scenarios representing the situations that might take place in market, have been defined. Scenarios are generated in terms of product price and demand change. Table 3-1 presents the scenarios, their definition and justification. Scenarios are illustrated graphically in Figure 3-3. As mentioned earlier, the FTL process can operate in different production modes, defined via three recipes; 55% diesel-45% wax shown in blue, 50% diesel-50% wax shown in red, and 45% diesel-55% wax shown in green.

Table 3-1 Market scenarios for the Thermochemical option

Scenario	Definition	Justification
Sc.1: Base case	Sinusoidal trend for price and demand of all products	Showing the volatility in the price and demand of products
Sc.2: Pessimistic	Price and demand of all products decline	Testing system's response in a situation in which market is weak
Sc.3: Optimistic	Price and demand of all products increase	Testing system's response in a situation in which market is strong
Sc.4	Diesel market grows, Waxes market crashes	Testing system's response in a situation when diesel market is stronger than wax market
Sc.5	Waxes market grows, Diesel market crashes	Testing system's response in a situation when wax market is stronger than diesel market

The assumptions for running the SC model for the manufacturing-centric policy are as follows:

- Process operates in one operating point in terms of production volume. The goal is to ensure minimizing production cost by running at the optimum operating point with minimum production cost (on a cost-per-unit basis).
- Process operates in one single production mode, i.e. the recipe does not change, and the fraction of FTL is fixed. The goal is to ensure minimizing production cost by producing the FTL fraction which yields with minimum production cost (on a cost-per-unit basis) and preventing changeover cost and time loss.

The assumptions for running the SC model for the margins-based policy are on the contrary, as stated below:

- The SC model is allowed to change the production volume to find the operating point that yields the highest profit.
- The SC model is allowed to change the production mode by changing the recipes based on market conditions.

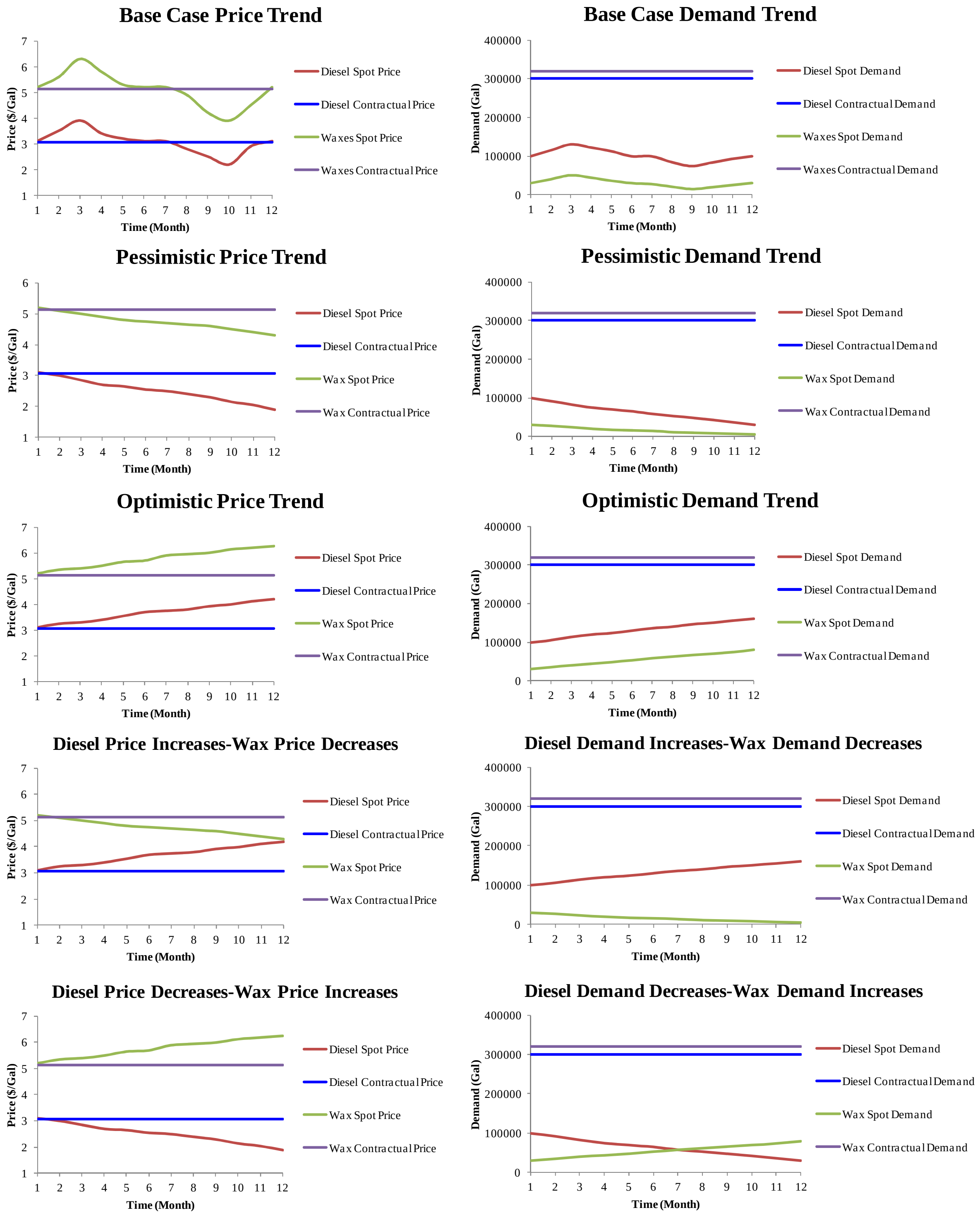


Figure 3-3 Market scenarios for the Thermochemical option

The SC model was run for both policies with their assumptions in case of all market scenarios. Because the recipe, representing production mode, cannot be changed for the manufacturing-centric policy, the SC model was run for two recipes in this case; 55% diesel-45% wax (blue) and 45% diesel-55% wax (green). The outcomes of the SC model for the base case scenario, showing the number of hours the process spent on each recipe and the production volume of each FTL fraction, for manufacturing-centric policy with green recipe and blue recipe, and margins-based policy are depicted in Figure 3-4, Figure 3-5, and Figure 3-6, respectively. It can be observed from the graphs that the production level is fixed and constant when manufacturing-centric approach is applied in the SC model and only one recipe is used deterministically. By contrast, both recipe and production level can change when applying margins-based approach.

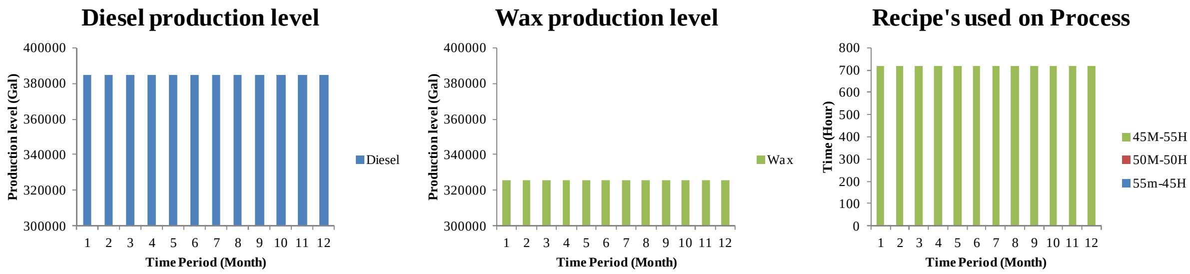


Figure 3-4 Manufactruign-centric(Green recipe):Production level and hours on each recipe

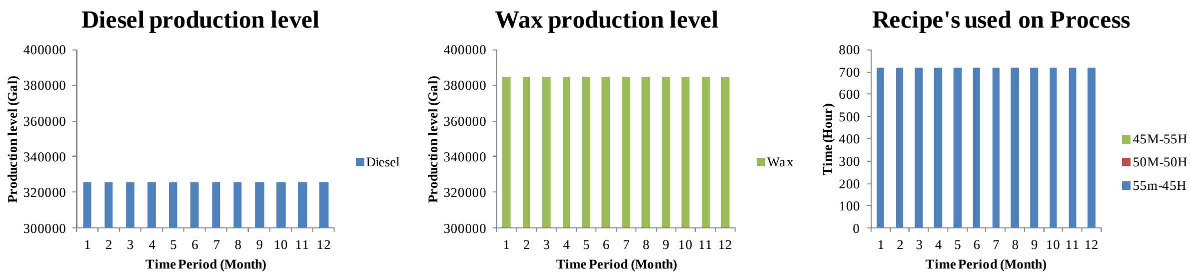


Figure 3-5 Manufactruign-centric (Blue recipe): Production level and hours on each recipe

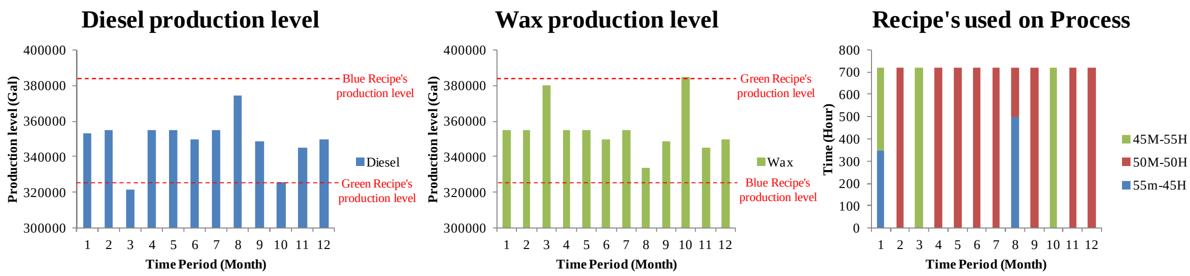


Figure 3-6 Margins-based policy: Production level and hours on each recipe (Base case)

The profit acquired by applying each policy is shown in Figure 3-7. As can be seen, the profit resulting from applying margins-based policy is higher than two other profits associated with the manufacturing-centric policy for all scenarios. The difference between the manufacturing-centric profits and margins-based profits are reported on the figure. In some scenarios, the difference is not significant, while in some other scenarios it is considerable. But the important point is that these improvements in profit due to applying margins-based policy are resulted from exploiting the inherent flexibility of the system. This means that no extra capital cost should be paid for this flexibility. Therefore, although the profit improvement is not very much significant, it is worth applying this policy, because, ultimately, there is no extra capital cost associated with that.

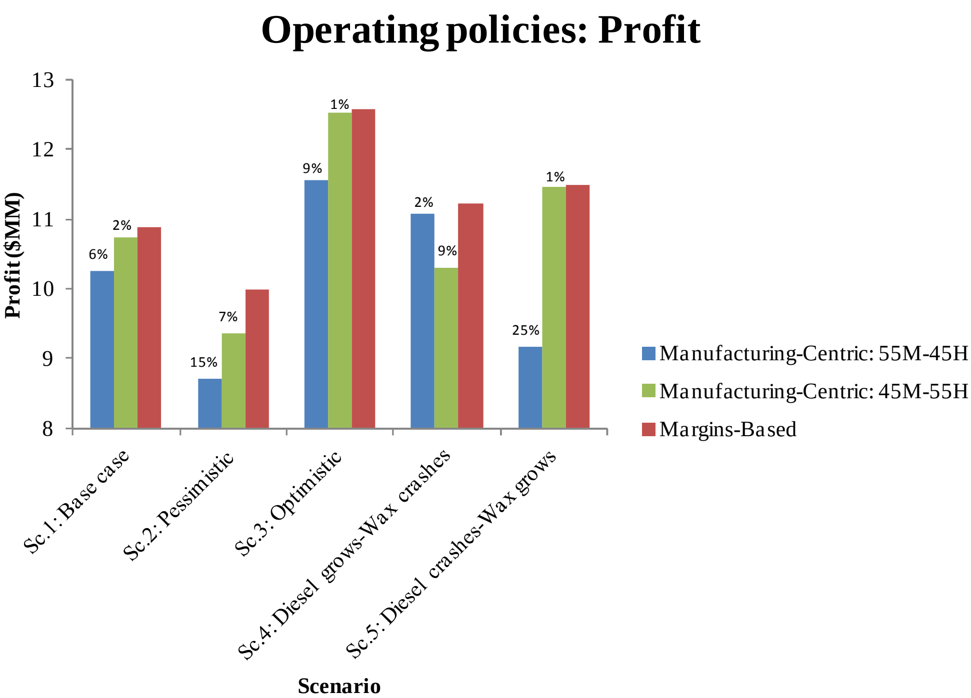


Figure 3-7 Profit resulting from applying both policies (Thermochemical option)

Figure 3-8 shows the production cost (excluding procurement cost) and revenue for both operating policies. Margins-based policy has a higher production cost than manufacturing-centric approach with blue recipe, which has the lowest production cost on a cost-per-unit basis, for all scenarios. But the revenue of margins-based approach compared to manufacturing-centric approach with blue recipe is much higher, resulting in higher profit in all scenarios. A different behavior is seen when comparing margins-based approach with manufacturing-centric approach with green recipe. The green recipe produces more of wax, as the most valuable FTL fraction, and may result in higher revenue, as it does in one scenario (Sc.2) compared to margins-based approach. But it has the highest production cost on a cost-per-unit basis, thus its total production cost in scenario 2 is much higher than that of margins-based approach. As a result, the profit of margins-based approach is higher. This means that margins-based approach maximize profit, either in some cases, by maximizing revenue though the production cost may also increase, or in some other cases, by minimizing production cost though the revenue may not be maximized. In all, margins-based policy tries to do a trade-off between revenue and production cost and to identify the perfect alignment between them to maximize profit.

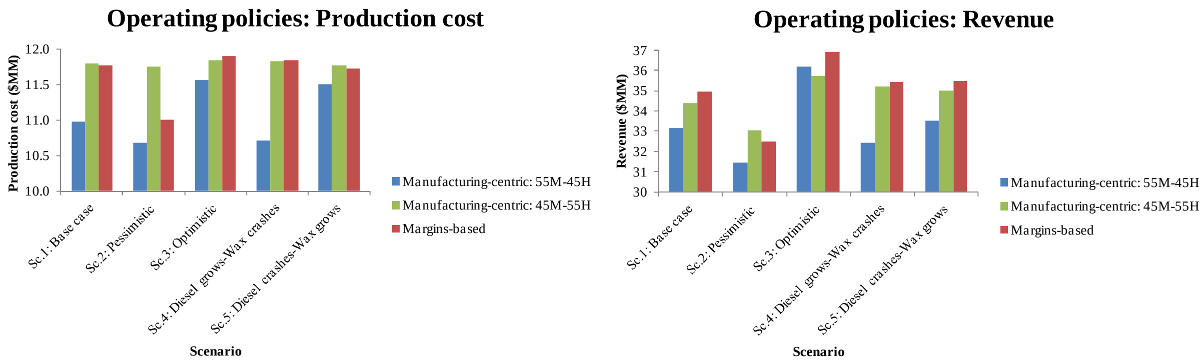


Figure 3-8 Revenue and production cost for both policies (Thermochemical option)

In these tests, the market demand was finite. The question remains to be answered is that what happens if market demand is infinite. A quick intuitive answer might be that by producing more of the most valuable product, i.e. wax, the profit will be maximized. Thus, there would be no need for the margins-based policy, and the manufacturing-centric approach with green recipe will result in the highest profit.

Some tests were carried out for this case. But in this case, as the market was infinite, price elasticity was taken into consideration, meaning that by putting more of a product into market, its price would shrink. Diesel is a commodity and its price elasticity is very low, while wax is a value-added product and has higher price elasticity. Due to lack of data, the value of price elasticity for wax was assumed to be -4.5. The results can be observed in Figure 3-9. In three scenarios, i.e. 1, 2 and 4, profit for the margins-based approach is slightly higher than that of manufacturing-centric approach with green recipe, while in two remaining scenarios the profit of both approaches are equal. The reason is that, even with an infinite market, producing wax may not be always profitable due to its price volatility and price elasticity. Figure 3-10 shows that, by applying the manufacturing-centric approach and producing more of wax, the company loses more than it gains, because its revenue on diesel decreases more than it increases in wax. It must be mentioned that the difference between profits in all scenarios is not considerable. That means if the price elasticity is lower, and the market is infinite, there will be a turning point in a price elasticity value in which the manufacturing-centric approach will yield the same result as the margins-based approach does.

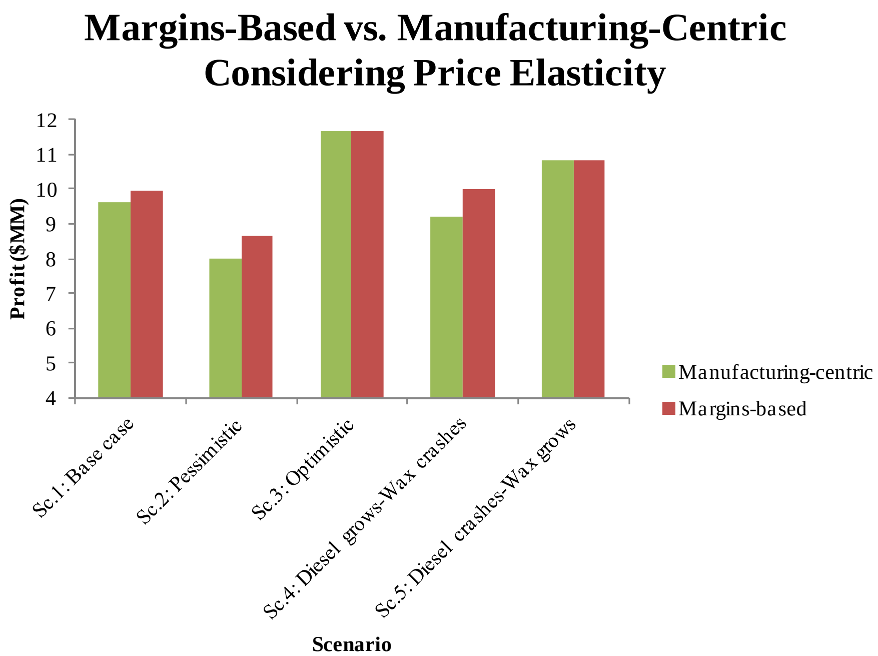


Figure 3-9 Profit of operating policies considering price elasticity

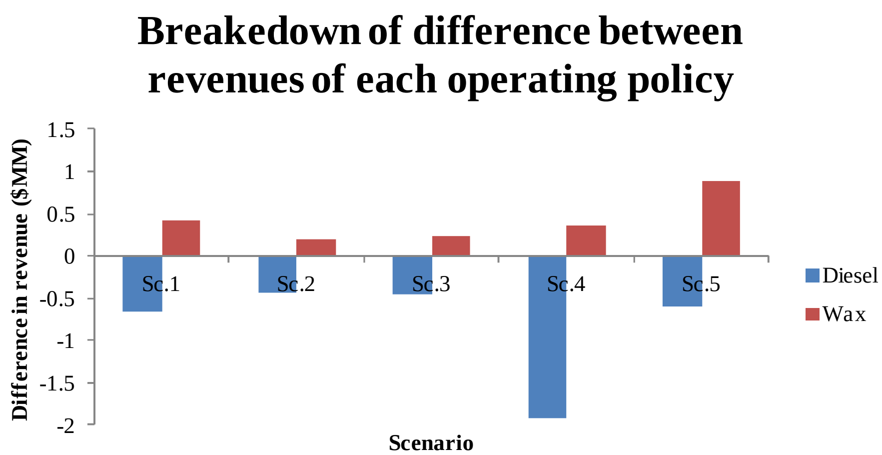


Figure 3-10 Difference between the revenues of manufactruing-centric and margins-based approaches: A breakdown

The SC model was run for three different price elasticities applying margins-based policy. Figure 3-11 illustrates the results. When price elasticity for wax is high (right side of figure), the margins-based policy mainly chooses the blue recipe more than others to produce more of diesel. When price elasticity is medium, the model tends to select the red recipe more to produce equal amount of both products. In case of low price elasticity, margins-based policy behaves like the manufacturing-centric approach and chooses the green recipe to produces more of the most profitable product, i.e. wax.

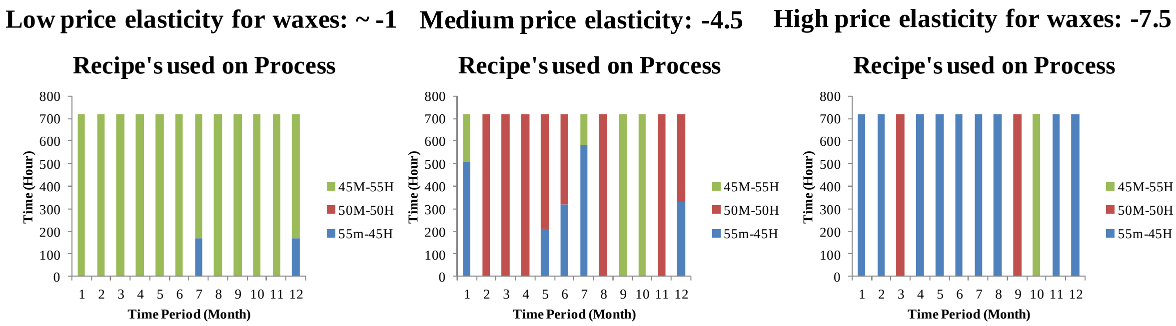


Figure 3-11 Recipes used on the process for different price elasticities

3.3.1.2 Biochemical option

The effect of employing both margins-based and manufacturing-centric operating policies was studied for the Biochemical option. The block flow diagram of the Biochemical option used in this part of the study is shown in Figure 3-12. First line operates in one production mode and produces LA. Second line operates in two distinct production modes, producing SA in one production mode and MA in the other production mode. Recipes are used to represent each production mode in the SC mathematical formulation. PLPW extraction has four recipes, one for each type of biomass. On the first line, fermentation process has only one recipe for LA, while the fermentation process of the second line has two recipes for SA and MA. Each line can also be shutdown. A recipe called "offline" is defined to show this operating mode. Changing from one recipe to another recipe implies changeover time and changeover cost.

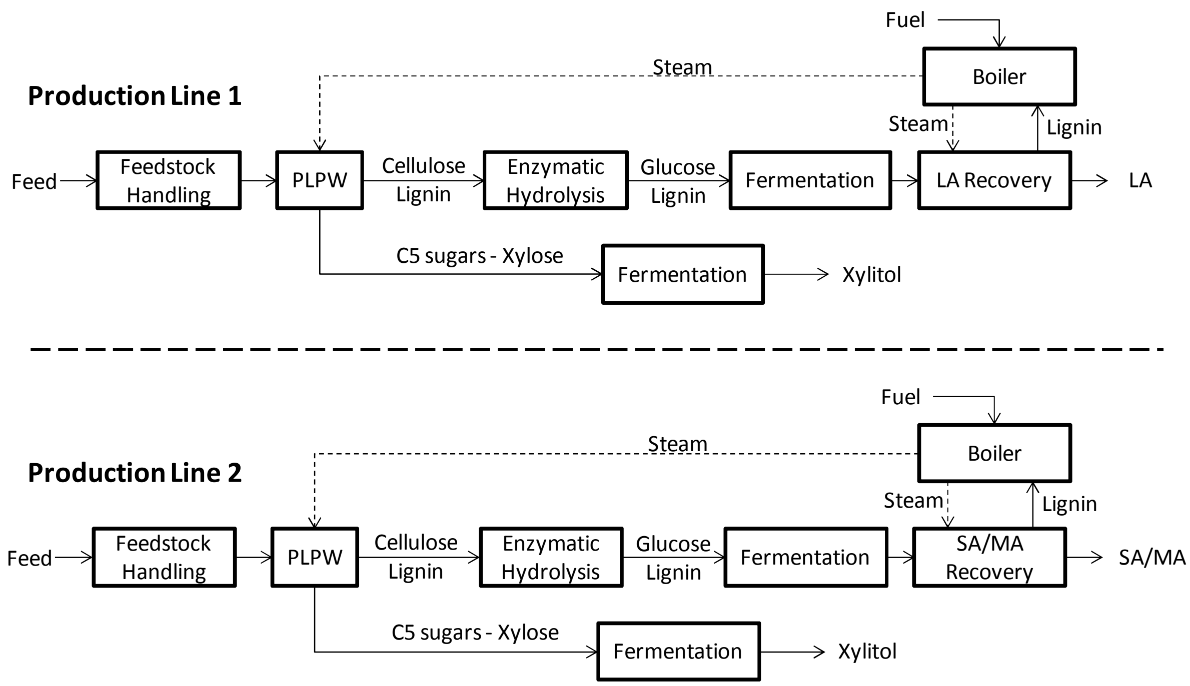


Figure 3-12 Block flow diagram: Biochemical option

Same tests were carried out for the Biochemical option to compare the result of applying margins-based and manufacturing-centric operating policies on the Biochemical option. There is more potential for flexibility in this option. In order to analyze the performance of this option in different market conditions, nine market scenarios representing the situations that might take place in market, have been defined. Scenarios are generated in terms of product price and demand change. Table 3-2 presents the scenarios, their definition and justification. Scenarios are illustrated graphically in Figure 3-13. As mentioned earlier, the second line in Biochemical option can operate in two different production modes, defined via two recipes; SA production shown in red and MA production shown in blue. There is another recipe shown in green, representing offline.

The assumptions for running the SC model for the manufacturing-centric policy are as follows:

- Process operates in one operating point in terms of production volume. The goal is to ensure minimizing production cost by running at the optimum operating point with minimum production cost (on a cost-per-unit basis).
- As the second line is flexible and needs a production sequence, a deterministic production sequence is defined to minimize the number of changeovers.

The assumptions for running the SC model for the margins-based policy are on the contrary, as stated below:

- The SC model is allowed to change the production volume to find the optimum operating point.

The SC model is allowed to change the production mode by changing the recipes based on market conditions to find the optimum production sequence.

Table 3-2 Market scenarios for the Biochemical option

Scenario	Definition	Justification
Sc.1: Base case	Sinusoidal trend for price and demand of all products	Showing the volatility in the price and demand of products
Sc.2: Pessimistic	Price and demand of all products decline	Testing system's response in a situation in which market is weak
Sc.3: Optimistic	Price and demand of all products increase	Testing system's response in a situation in which market is strong
Sc.4	MA market grows, SA and LA market crash	Testing system's response in a situation when MA market is stronger than SA and LA markets
Sc.5	SA market grows, MA and LA market crash	Testing system's response in a situation when SA market is stronger than MA and LA markets
Sc.6	LA market grows, MA and SA market crash	Testing system's response in a situation when LA market is stronger than MA and SA markets
Sc.7	MA market crashes, SA and LA market follow the base-case trend	Testing system's response in a situation when MA market is weaker than SA and LA markets
Sc.8	SA market crashes, MA and LA market follow the base-case trend	Testing system's response in a situation when SA market is weaker than MA and LA markets
Sc.9	LA market crashes, SA and MA market follow the base-case trend	Testing system's response in a situation when LA market is weaker than SA and MA markets

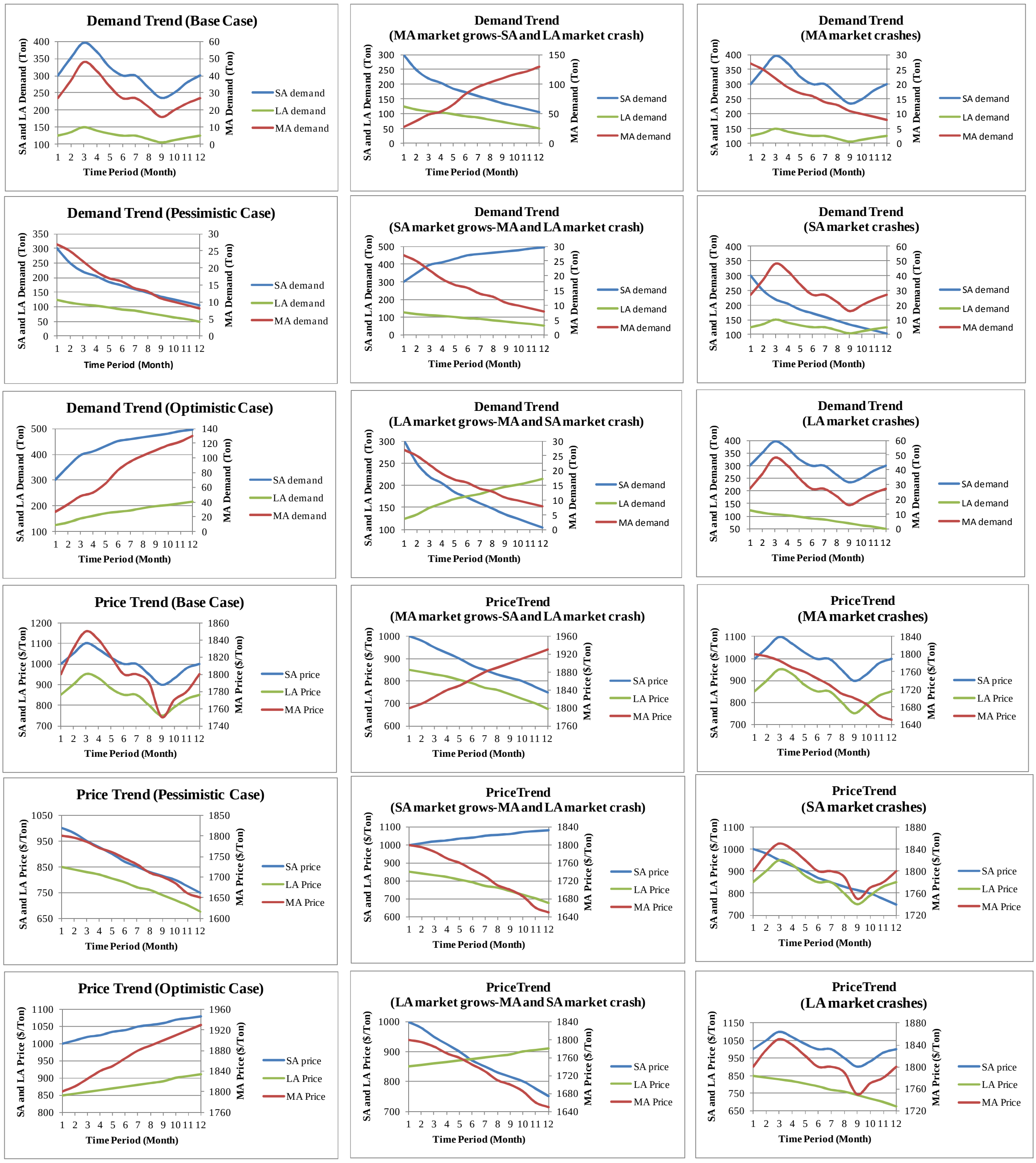


Figure 3-13 Market scenarios for the Biochemical option

The SC model was run for both policies with their assumptions in case of all market scenarios. The first line is dedicated to LA production, while the second line can produce SA and MA. Thus, the recipe can be changed in the fermenter of the second line. The outcomes of the SC model for the base case scenario, showing the production sequence of second line fermenter for manufacturing-centric policy and margins-based policy are depicted in Figure 3-14.

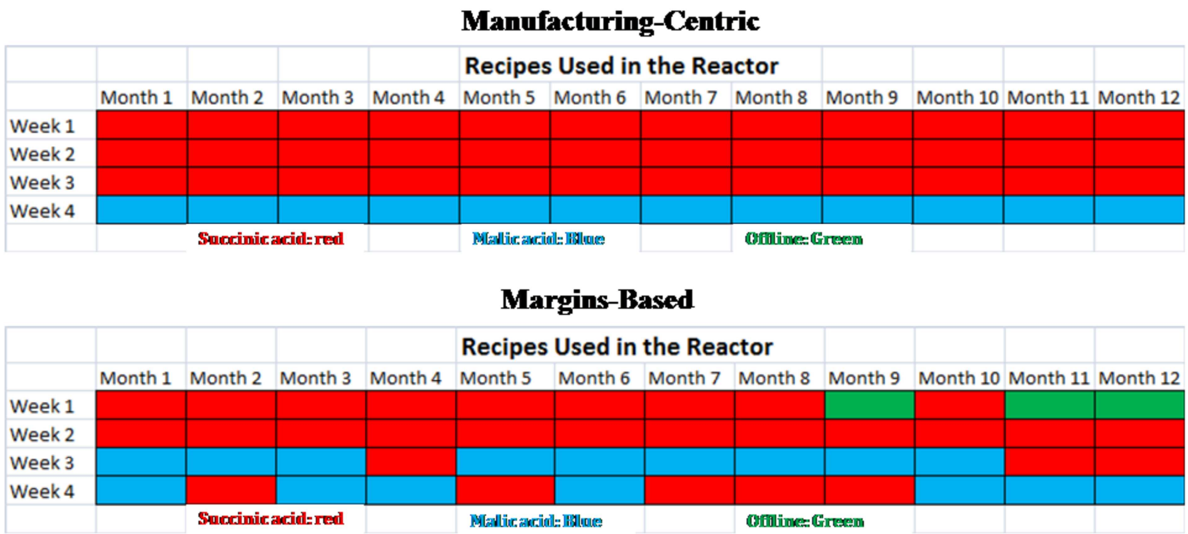
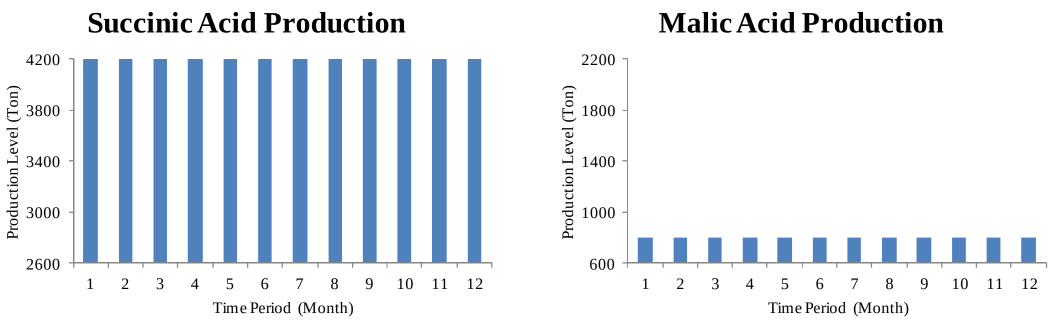
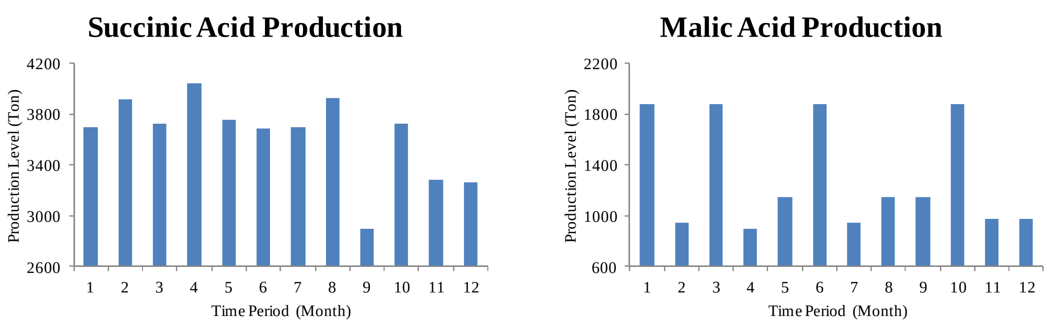


Figure 3-14 Recipes used in second fermentor for both operating policies (base cas)



Production volume in second fermentor: Manufacturing-centric approach (base case)



Production volume in second fermentor: Margins-based approach (base case)

Figure 3-15 Production volume in second fermentor for both policies

It is seen that the SC model chooses a different sequence of recipe compared to the deterministic sequence used in the manufacturing-centric approach, and in some periods, process was shutdown (represented by offline recipe in green). Figure 3-15 depicts the production level of each product in the second fermentor for both policies for base case market scenario. Production level in manufacturing-centric approach is uniform, while in margins-based approach the production level changes based on market conditions.

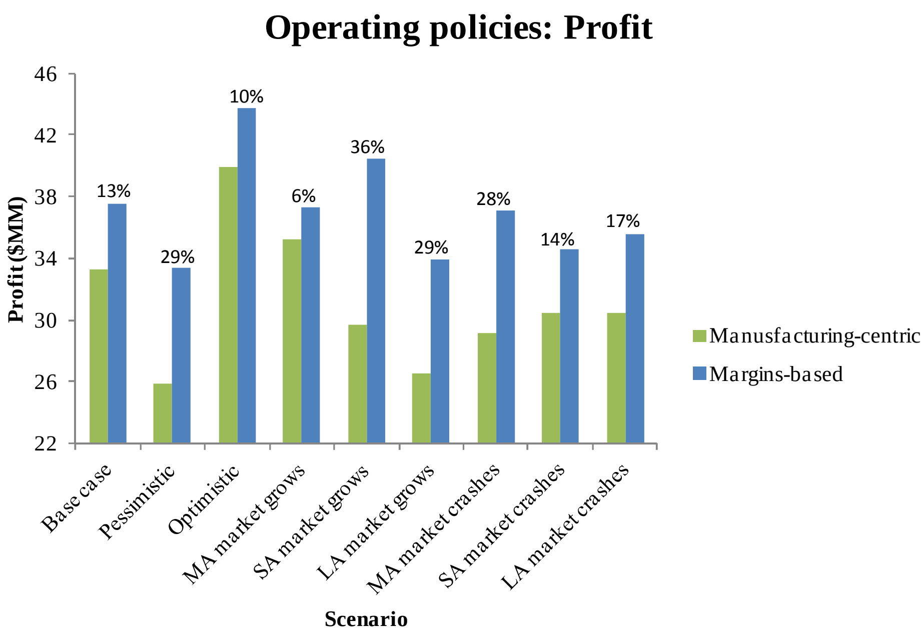
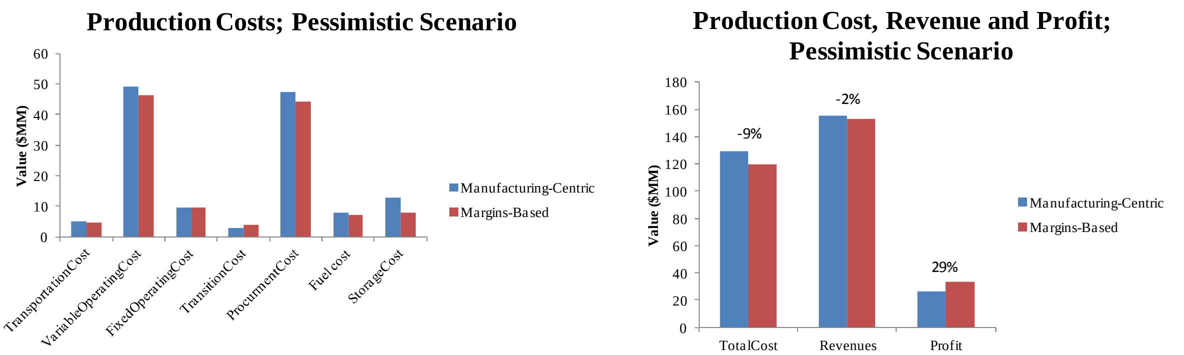


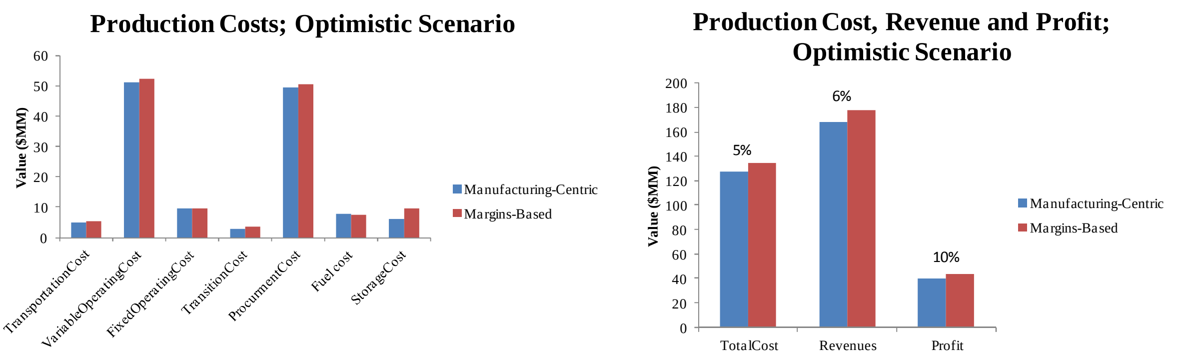
Figure 3-16 Profit resulting from applying both policies (Biochemical option)

The profit acquired by applying each policy is shown in Figure 3-16. As can be seen, the profit resulting from applying margins-based policy is significantly higher than the profits associated with the manufacturing-centric policy for all scenarios. The difference between the manufacturing-centric profits and margins-based profits are reported on the figure. Unlike the Thermochemical option, it can be seen that the profit improvements for all scenarios are quite significant. As mentioned before, the Biochemical option produces value-added products and following the market needs by applying margins-based policy has much more significant impact on profit improvement compared to the Thermochemical option. Again, the important point is that the improvements in profit due to applying margins-based policy are resulted from exploiting the inherent flexibility of the system and no extra capital cost is associated with this flexibility.

Figure 3-17 shows the production costs in detail, and total production cost, revenue and profit for two extreme scenarios, i.e. pessimistic and optimistic. Figure 3-17.a illustrates that, for the pessimistic case, all production costs for margins-based policy is lower than those of manufacturing-centric approach, except changeover (transition) cost. As can be seen on the right side, although the revenue of margins-based approach is lower, its total cost is much lower, resulting in a higher profit. This demonstrates that the margins-based policy has declined some orders, and because of that its revenue is lower, but has decreased the production cost too, so that the profit is higher compared to manufacturing-centric approach. This means that some orders that have been fulfilled by the manufacturing-centric approach were not profitable. A higher changeover cost for the margins-based policy implies that the SC model identifies the most profitable orders and change the recipe to fulfill those orders. It is clear that the changeover cost is very well paid off. Figure 3-17.b depicts the same result for the optimistic case. In the optimistic scenario market is strong and the whole capacity is used and thus all production costs of margins-based approach are higher than those of manufacturing-centric approach. On the other hand, the revenue increases more, and therefore the final profit for the margins-based approach is higher.



(a) Biochemical option (Pessimistic scenario)



(b) Biochemical option (Optimistic scenario)

Figure 3-17 Production cost breakdown, total production cost, revenue and profit

3.3.1.3 Conclusion

In the P&P industry, the current manufacturing culture is toward cost minimization. It is believed that production costs play the major role in profit. Revenue management practices are ignored and revenue is considered as a fixed component in profit calculations. Using a margins-based policy, revenue is seen as a master component to cost that must be maximized to maximize the overall profit. It can be concluded that margins-based policy can improve the profit of a biorefinery by identifying the optimum alignment between revenue and costs to maximize profit:

- It improves profit by either increasing revenue, e.g. in case of strong market, or decreasing cost, e.g. in case of weak market.
- The profit improvement for added-value chemicals is significant, whereas for commodities is not considerable.
- But even for commodities, this policy is worth applying as there is no cost associated with that.
- It must be mentioned that, in case of low price elasticity and a large market, the result of margins-based approach is similar to the manufacturing-centric approach.

3.3.2 Metrics for evaluating the biorefinery supply chain performance

As mentioned in the methodology section of this thesis, there are three metrics used in the methodology to evaluate the performance of designed SC in different market conditions; SC profitability, robustness and flexibility. These metrics are directly employed for decision making in this work. Moreover, a conditional value-at-risk (CVAR) parameter is introduced to analyze levels of risk in making sales decisions and to provide required information for profit-risk trade-offs. The work related to CVAR is not a part of the proposed methodology, but provides opportunities for future works.

For sustainable decision-making regarding biorefinery strategies, criteria from different perspectives, i.e. economic, environmental and social, should be considered. Thus, several metrics from different tools are required for quantifying the performance of a strategy. Economic metrics that are used in decision making, which are mainly related to the profitability of a strategy, are incapable of accounting for the market volatility (Hytonen & Stuart, 2011), whereas today's market is subject to volatilities in terms of price and demand and it is critical that biorefinery strategies are flexible in order to be robust to market volatility. Sensitivity analysis is typically executed to address the impact of possible market scenarios on profitability. Even in this case, the problem is viewed as a steady-state case and the dynamism of the market, i.e. changes in price and demand over the given time period, are ignored. Moreover, it is not easy to use the result of a sensitivity analysis in an MCDM framework. Instead, it is desirable to reflect the response of a strategy to such dynamism by relevant metrics. This part of the work presents metrics for SC profitability, flexibility and robustness that can be used in an MCDM framework, in conjunction with economic criteria, for the evaluation of the FBR process options and SC strategies.

3.3.2.1 Supply chain profitability

There are several profitability estimation methods that can be used to estimate the profitability of a project. From a generic perspective, these methods can be divided into two main groups; methods that do not consider the time value of money, which include the rate of return on investment (ROI), payback return, and net return, and methods that consider the time value of money, which include the discounted cash flow rate of return, simply called internal rate of return (IRR), and net present value (NPV) (Peters & Timmerhaus, 2003). In this work, ROI and IRR are used as profitability metrics. ROI does not consider the time value of money, variable depreciation allowance, increasing maintenance costs over the project life, or changing sales volumes, but it is a simple measure which is generally used for preliminary design calculations. IRR considers time value of money as well as depreciation. It is an ideal metric for the projects that are going to be implemented over time through several phases. For such projects considering the profitability in the long run is of crucial importance.

Generally in economic analyses, the profitability measures consider the costs incurred by the process. Some SC-related costs such as procurement cost and transportation cost are taken into account in profitability calculations, but some other costs, which are related to the dynamism and volatility of the production environment such as inventory cost and changeover cost, are typically ignored. The SC profitability metrics used in this study consider all cost contributors to provide a better cost representation at the decision-making level.

3.3.2.2 Metric of robustness (MR)

In a robust design the control parameters of a system are selected in such a way that the desirable measured function do not diverge significantly from a given value (Bernardo, Pistikopoulos, & Saraiva, 1999). Klibi et al. (2010) define robustness of an SC network as the extent to which the network is able to carry its functions for a variety of plausible future scenarios. In this work, robustness is not considered in the optimization formulation, meaning that the robustness of the system is not optimized. Instead, a metric of robustness (MR) is used to quantify the robustness of design options against market volatility so that design options can be compared in terms of robustness. Several robustness metrics have been introduced thus far (Vin & Ierapetritou, 2001). Well-known metrics are standard deviation and mean absolute deviation (Bernardo, Pistikopoulos, & Saraiva 2001). For the sake of simplicity and interpretability for an MCDM panel, a simple formulation is used as robustness metric, as shown in equation 40.

$$MR = \left(\frac{\sum_{N_{Sc}}(Pr_B - Pr_{Sc})}{Pr_B}\right)^{-1} \qquad (40)$$

where Pr_B is the base case profit, Pr_{Sc} is the profit for scenario Sc and N_{Sc} is the number of scenarios. In this work, the desired parameter that must not diverge from a given value is profit. It is desirable that the profit of a design option in case of each market scenario does not deviate from the base case profit, if this profit is lower than the base case profit. Therefore, to quantify the downside risk of volatility, calculated profits that are less than the base case profit are considered in this equation. The MR shows the percentage of aggregate deviation from the base case profit for all profits that are less than the base case profit. The smaller this percentage is the better and more robust the system will be. Hence, the reverse of the percentage is used, so that the metric shows higher values for more robust systems. This metric implies that the lower the deviation of the downside profits from the base case profit is, the more robust the system will be.

The classic robustness metrics that somehow calculates an average deviation from the desirable value cannot consider the number of downside scenarios. A case with one downside scenario whose profit deviates $1MM from the base case profit has the same standard deviation compared to a case with, for instance, five downside scenarios whose profits also deviate $1MM from the base case profit. Therefore, in the proposed metric, the aggregation of downside profit was considered.

3.3.2.3 Metric of flexibility (MF)

As mentioned in the literature review section, the concept of manufacturing flexibility in the FBR implies the ability to produce several bioproducts (product flexibility) at different volumes (volume flexibility) and in different time periods based on product price and demand. In the design of chemical processes, volume flexibility has a critical role. Thus, in order to design or analyse the flexibility of a system, quantifying volume flexibility is of crucial importance. Inspired by the work of Voudouris (1996) on qualitative measure of flexibility, metric of flexibility (MF) quantifies volume flexibility, as shown in equation 41:

$$MF = \sum_p \sum_m \frac{\sum_t \left| C_{mpt} - C_{mp}^N \right|}{\sum_t C_{mp}^N} \qquad (41)$$

where $\mathrm{C_{mpt}}$ is the amount of product *m* that is produced on process *p* in time period *t* and $\mathrm{C_{mp}^N}$ is the amount of product *m* produced on process *p* by the nominal production rate over the same number of processing hours. This formulation shows the deviation from the nominal production rate in a dimensionless form and implies volume flexibility.

Three process alternatives from Thermochemical option and two process alternatives from the Biochemical option are considered to test the metrics. Each alternative has a specific potential for flexibility. These process alternatives are explained in details in the next part of the methodology, as they are defined through that part. For this step, it is just assumed that these alternatives are associated with a specific potential for flexibility, as presented in Table 3-3.

Table 3-3 Process alternatives with different potential for flexibility

Alternative	Flexibility
Thermochemical option	
A-1 A-2 A-3	Low flexibility Medium flexibility High flexibility
Biochemical option	
B-1 B-2	Low flexibility High flexibility

The SC model was run for all nine scenarios defined for each option. The results for the Thermochemical option and Biochemical option are presented in Figure 3-18 and Figure 3-19, respectively. It can be seen on the left-hand side of both figures that as the potential for flexibility increases, the profit increases in all market conditions. On the right-hand side, it is shown that as the potential for flexibility increases in each portfolio option, more flexibility is used, i.e. the average flexibility used by each alternative increases as the flexibility potential of that alternative increases. Moreover, it can be seen that by using more flexibility the robustness improves for both options.

Another important observation is that the profitability does not necessarily increase with flexibility. This is because the fact that increase in revenue due to having more flexibility cannot compensate the increase in capital costs. It can be seen that profit increases with flexibility for all cases. But in Thermochemical option, although A-3 is more flexible than A-1 and A-2 and has more profit, its ROI is less. Therefore, in the case of Thermochemical option, the flexibility cannot be justified. Biochemical option has a different behavior. Alternative B-2 leads to a higher profit and profitability compared to B-1. Thus, it can be concluded that, for this option, the extra capital spent for flexibility can very well be paid off.

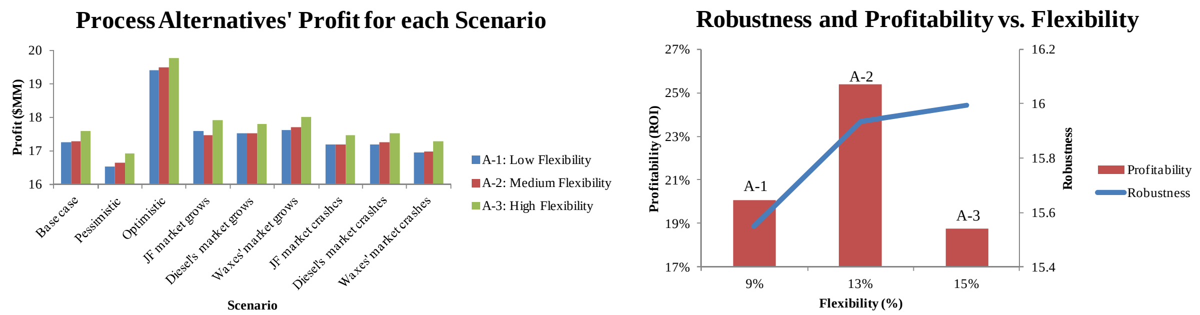


Figure 3-18 Profit, profitability and robustness for different flexibility potentials: Thermochemical option

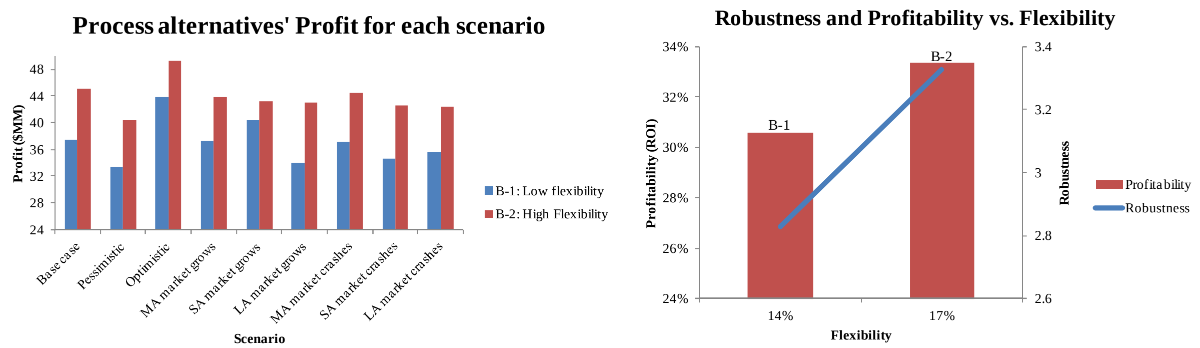


Figure 3-19 Profit, profitability and robustness for different flexibility potentials: Biochemical option

To sum up, using simple metrics that are developed, the robustness and the flexibility of the system can be quantified. As it is not obvious whether by increasing flexibility, profitability would increase or not, such metrics can be utilized for doing a trade-off, i.e. it can be shown to what level of flexibility, profitability improves. Moreover, the effect of increasing flexibility on the robustness of the system can be investigated. It was shown that increasing flexibility will make the system more robust to market volatility. In fact, in a volatile market, a more flexible system can change its production volume and align it with the market demand. It can also swing from the production of one product, which is less profitable, to the production a more profitable product. Therefore, the capability of the system for flexibility can be exploited so that the maximum possible profit can be obtained by the system. Overall, such metrics can very well quantify the operational performance of s system in terms of flexibility and robustness.

3.3.2.4 Conditional value-at-risk (CVAR)

As discussed by Verderame and Floudas (2011), CVAR aims at guarding against realization of uncertain parameters by going beyond the expected evaluation when expressing the uncertainty of system parameters. A loss function must be defined as a function of decision vector and uncertain parameters with a probability distribution. Using the loss function and the acceptable loss level, two constraints are added to the optimization formulation which restrict the evaluation of the system's variables according to a user-specified risk-aversion parameter.

Inspired by (Verderame & Floudas, 2011), a CVAR-like parameter was added to the SC formulation. Contractual order acceptance percentage (OA) is considered to study the risk associated with acceptance/rejection of the contractual orders. A high OA implies less risk, because contractual orders are fixed in price and amount over the long term and thus they can secure the profit. On the other hand, a low OA connotes more spot orders which might improve the profit, as spot prices are sometimes higher than the contractual prices, but poses higher risks, because spot demands are not certain. A constraint is added to the optimization formulation, in which OA should be bigger than a risk factor. Probability of market scenarios are not considered in this study. The added constraint is shown in equation 42:

$$\frac{\textit{Volume associated with the accepted contractual orders}}{\textit{Volume associated with all contractual orders}} > \alpha \quad (42)$$

where α is the risk parameter.

For this part of the work, only the Biochemical Option was considered. Market scenarios defined previously in Table 3-2 and Figure 3-13 are modified slightly. Market scenarios represent only price volatility, and demand changes follow the base case demand trend. In this way, a specific OA value means one order acceptance pattern for all market scenarios, while, if the demand trend changes in each scenario, an OA value will be associated with a different order acceptance pattern for each scenario, and hence, the results of different scenarios cannot be compared. A worst case scenario is also added to the market scenarios. In this scenario, the spot market is very weak. This scenario is generated to show the risk of rejecting contracts when spot market is weak.

Table 3-4 shows the result of CVAR study. SC model was run for market scenario 1, 2, 3, 4, 5, 7, 8 and worst-case scenario. The profit was calculated for several levels of OA. Profits are shown in $MM. It can be seen that the maximum profit happens in different percentages (highlighted in bold), showing that there is not one optimum OA for all scenarios. In 80% OA, the average profit and the robustness metric has the highest value, except compared to the 100% OA which has a low profit, but the best robustness. Therefore, 80% OA can be chosen over lower OAs, and then be compared to 100% OA. Decision makers with low risk tolerance may choose 100% OA which has better robustness, while those with higher risk tolerance can choose 80% OA which has the highest profit. The results are shown in Figure 3-20 and Figure 3-21, graphically.

Table 3-4 Profit, robustness and average profit for Biochemical option in case of different OAs and market scenarios

OA%	Sc.1	Sc.2	Sc.3	Sc.4	Sc.5	Sc.7	Sc.8	Worst	MR	Average Profit
22.03%	37.57	34.16	40.32	34.33	38.27	37.47	34.25	7.66	0.93	33.01
28.81%	39.52	36.11	42.27	36.28	40.22	39.43	36.21	9.28	0.98	34.92
49.15%	45.08	42.08	**47.77**	42.25	45.86	44.98	42.17	16.33	1.19	40.82
50.85%	45.16	42.29	47.77	42.46	**45.92**	45.06	42.38	16.87	1.22	40.99
72.88%	**45.19**	44.36	45.97	44.53	44.43	**45.09**	44.46	24.16	1.93	42.28
79.66%	45.17	**44.80**	45.52	**44.97**	44.28	45.07	**44.90**	25.95	**2.24**	**42.59**
100.00%	35.94	35.35	38.33	35.35	36.12	35.94	35.35	**34.00**	**9.74**	**35.80**

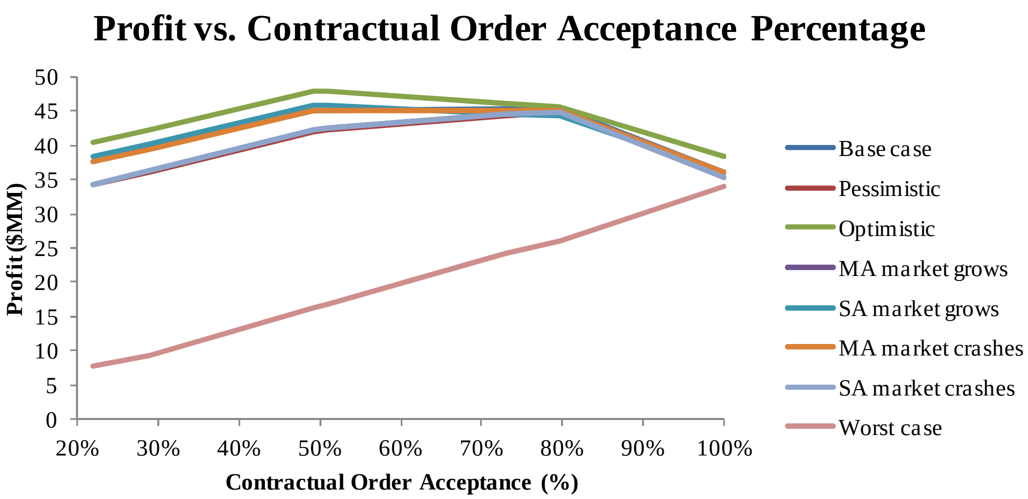


Figure 3-20 Profit vs. OA

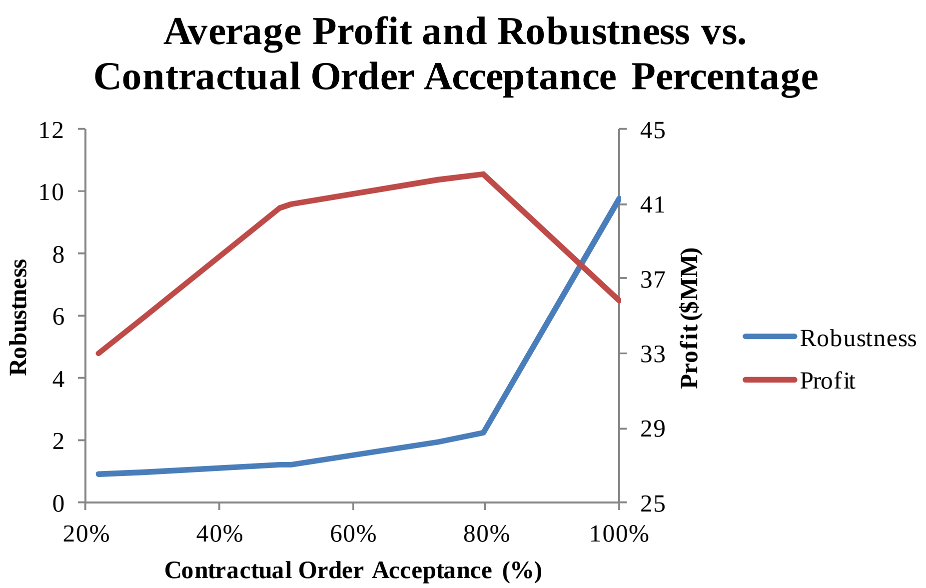


Figure 3-21 Average profit and robustness vs. OA

Figure 3-22 demonstrates the percentage of the accepted orders resulted in the highest profit for each scenario. For the optimistic scenarios (3 and 5), the maximum profit happens in lower OAs compared to other scenarios, because in these scenarios the spot market is strong and more spot orders are fulfilled and lower OA results in higher profit. By contrast, for pessimistic scenario (2) and scenarios with declining trends (4, 7 and 8), more contracts are accepted and fulfilled, because the spot market is weak. For the worst case scenario, the maximum profit is acquired at 100% OA, because the spot market is not profitable at all and at 100% OA, where all contracts are made, the profit is maximized. Figure 3-23 reveals how production capacity is dedicated to spot and contractual orders for the OAs resulted in the highest profit. For the optimistic scenarios more capacity is dedicated to spot orders. On the contrary, for other scenarios the capacity dedicated to contractual orders is bigger.

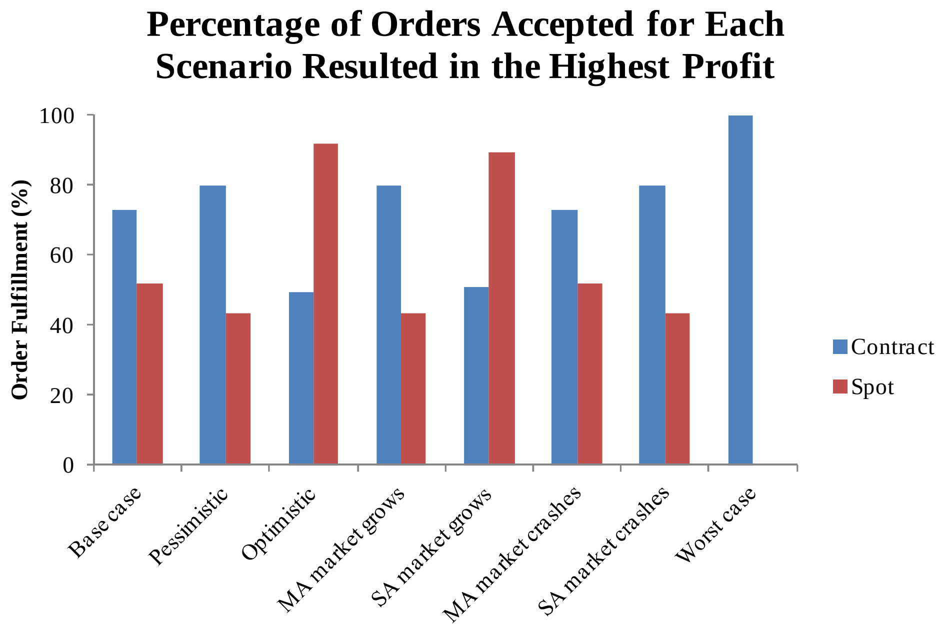


Figure 3-22 OA for spot and contractual orders

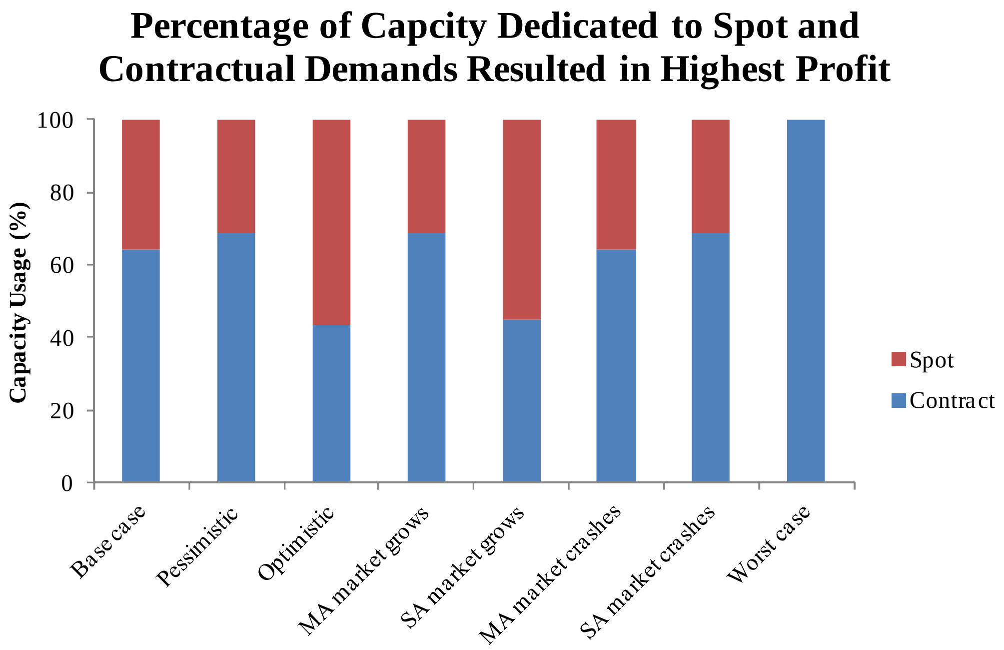


Figure 3-23 Capacity utilization for spot and contractual orders

3.3.2.5 Conclusion

Metric of flexibility and metric of robustness can give a good insight on how a SC reacts against market volatility. Such metrics can quantify the performance of SC at the operational level in different market conditions. Therefore, they can be used for, either targeting the design of a system by identifying the best design based on its operational performance, or comparing different alternatives by comparing their operational performances. Furthermore, CVAR studies show that optimum contractual percentage of order acceptance is different for each market scenario. This study demonstrates that lower risks may imply lower profit and thus, an appropriate trade-off analysis ought to be performed to choose the right OA.

In the next part of the methodology, these metrics are used to quantify the behavior of different systems against several market conditions. As each metric represents a specific capability of the system, they can be used to evaluate different design alternatives.

3.3.3 Targeting the level of flexibility

In this section, the results of targeting the level of flexibility and designing the SC network are presented. Based on mill's assessments, 1000 bone-dry tons per day of woody biomass can easily be available in the region. Their market assessment targets an FTL process requiring 500 bone-dry tons per day of woody biomass for the Thermochemical option, and an acid production system requiring 1000 bone-dry tons per day of woody biomass for the Biochemical option.

The characterization of options is presented in Table 3-5. This characterization helps to define design alternatives representing different flexibility potentials in the next step.

Table 3-5 Process characteristics for each option

Portfolio option	Characteristics
Thermochemical FTL to waxes and diesel+ diesel to Jet fuel	Type of process: Continuous Process configuration: Lines in series Product flexibility: Each line produces only one product Volume flexibility: Each process has 5% volume flexibility The fraction of wax and diesel can change from 45%–55% to 55%–45%
Biochemical Lactic acid, Succinic acid, Malic acid	Type of process: Semi-continuous (Batches in series) Process configuration: Lines in parallel Product flexibility: All products can be produced in similar fermenters, but in different modes. They need specific recovery systems Volume flexibility: Each process has 5% volume flexibility

Following the discussions with mill board of executives, three process design alternatives were defined for the Thermochemical option. Process alternatives representing different flexibility potentials for the Thermochemical option are illustrated in Figure 3-24. In the first alternative, A-1, FTL is separated into waxes and diesel. The waxes are sold, and the whole diesel is converted to JF using hydro-treating process. In the second alternative, A-2, a smaller process is used to convert diesel to JF. Hence, this system has more potential for flexibility in terms of product, because wax, diesel and JF can be produced at the same time. The hydro-treating process can be shutdown if JF market is weaker than the diesel market. The third alternative is a combination of A-1 and A-2. Two small hydro-treating processes are used in parallel. If both are in operation, the system performs like A-1 and if one of them is shut down, it performs like A-2. This alternative has the highest potential for flexibility.

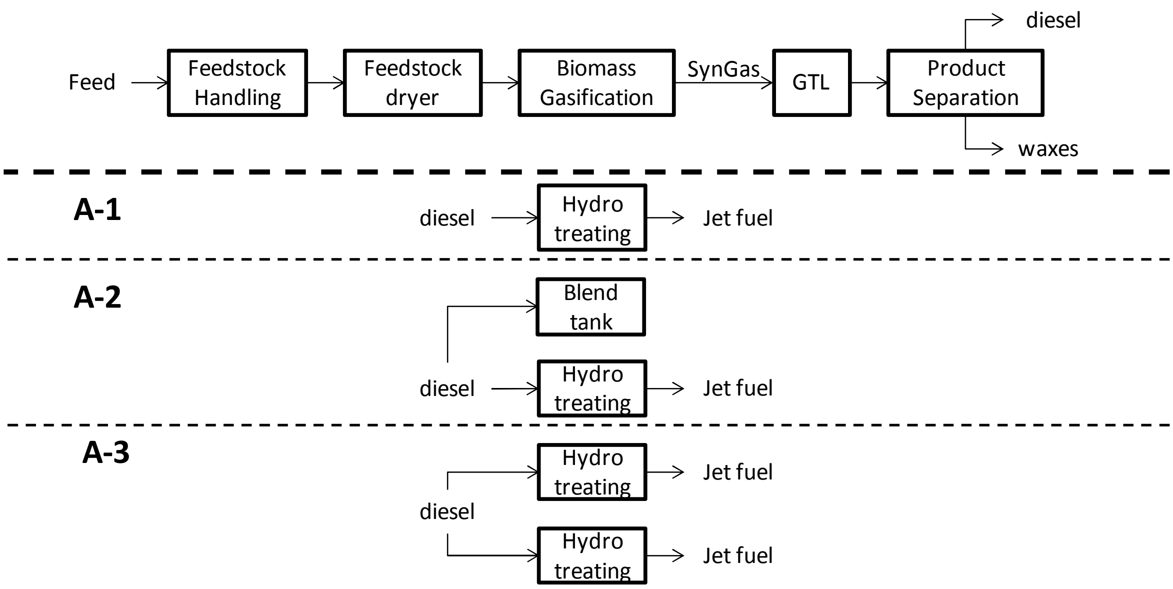


Figure 3-24 Process alternatives: Thermochemical option

For the second portfolio, two process alternatives have been considered, as shown in Figure 3-25 and Figure 3-26. In the first alternative, B-1, there are two separate lines. The first line produces LA and the second line produces SA and MA in different production modes. As mentioned before, all processing steps up to the recovery systems are similar in both lines. Thus, in the second alternative, an SA/MA recovery system, highlighted in red in the figure, is added to LA production line, so that this line can be changed over to produce SA or MA as well. One of SA/MA and LA recovery systems is always in standby mode. Hence, second alternative has more potential for flexibility.

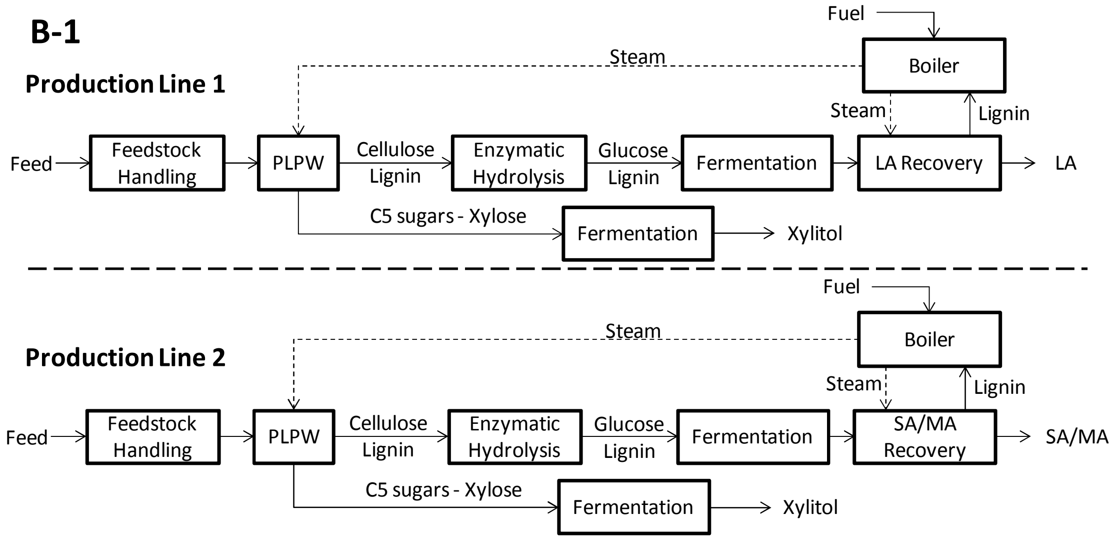


Figure 3-25 Process alternatives: Biochemical option (B-1)

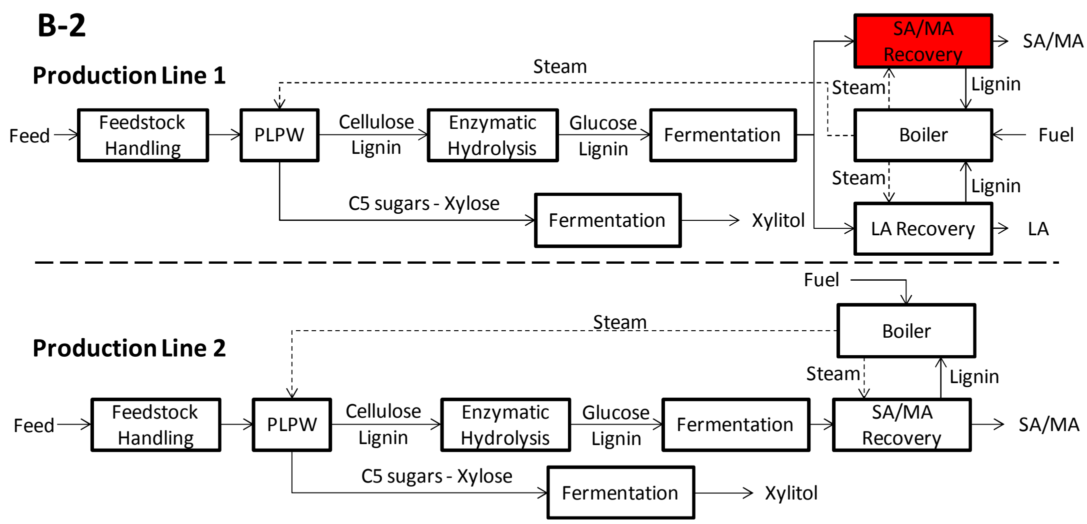


Figure 3-26 Process alternatives: Biochemical option (B-2)

After defining process alternatives, SC network alternatives must be defined and combined with the process alternatives. Table 3-6 and Table 3-7 show the SC network alternatives defined for the each portfolio option. Company's restrictions and policies must be considered in the definition of the SC network alternatives. Therefore, different processing, selling, transportation and partnership strategies shown in these tables are defined by the mill's executives. Thermochemical option, which has three process alternatives, has six SC network alternatives. Each process alternative is associated with two SC network alternatives. Biochemical option has two process alternatives. Two SC network alternatives are associated with each of them, making four SC network alternatives in total.

The SC networks are defined considering the process options. For process alternative A-1, which can potentially convert the whole diesel into JF, there are two SC network alternatives at the processing stage; either making partnership with a JF producer which in turn implies a specific selling strategy for diesel, i.e. selling diesel completely to JF producer, or producing JF at the mill. For process alternative A-2, which can produce both diesel and JF, there are two SC networks alternatives at the sales level for diesel; either making a contract with a partner and sending diesel to him, or selling it on the spot. For process alternative A-3, there are two SC network alternatives at the transportation level for wax and diesel; either buying trucks or making contract with a transportation company.

For process alternative B-1 and B-2, SC network alternatives are different at processing level. There are two alternatives; either sending the extractives (hemicelluloses and C5 sugars) to a partner for more processing, or processing them at the mill. Moreover, different transportation strategies can be defined.

Table 3-6 SC network alternatives for Thermochemical option

	A-1	**A-2**	**A-3**
Processing	Partnership with JF producer OR Producing JF at the mill	Producing JF at the mill	Producing JF at the mill
Selling	Waxes: Contract & Spot Diesel: To JF producer OR To be converted to JF Jet fuel: Contract	Waxes: Contract & Spot Diesel: Contract with a partner OR Spot Jet fuel: Contract	Waxes: Contract & Spot Diesel: Contract & Spot Jet fuel: Contract & Spot
Warehousing	Expansion	Expansion	Expansion
Delivery/ Transportation	Wax delivery Buy trucks Partnership for JF delivery	Wax and diesel delivery Buy trucks Partnership for JF delivery	Wax and diesel delivery Buy trucks OR Contract with a partner Partnership for JF delivery

Table 3-7 SC network alternatives for Biochemical option

	B-1	B-2
Processing	Send extractives to partner OR Process extractives at the mill	Send extractives to partner OR Process extractives at the mill
Selling	SA: Contract & Spot MA: Contract & Spot LA: Contract & Spot	SA: New market for Contract & Spot MA: Contract & Spot LA: Contract & Spot
Warehousing	Expansion	Expansion
Delivery/ Transportation	Buy trucks OR Contract with a logistics partner	Partnership for SA delivery/selling For other products: Buy trucks OR Contract with a logistics partner

The total capital investment required for each combined alternative is shown in Table 3-8.

Table 3-8 Capital investment of combined alternatives

Portfolio 1			Portfolio 2		
Process alternative	SC network alternative	Capital ($MM)	Design alternative	SC network alternative	Capital ($MM)
A-1	Partner for JF	61	B-1	Sell extractives	113
	Produce JF	87		Process extractives	122
A-2	Diesel on spot	78	B-2	Sell extractives	122
	Partner for diesel	76		Process extractives	131
A-3	Buying trucks	98			
	Partnership	95			

SC optimization model is run for different operating windows (different levels of flexibility) of each alternative in case of all market scenarios. The result of this step is shown for alternative B-1 in Figure 3-27, Figure 3-28 and Figure 3-29. As can be observed in Figure 3-27, profit improves with increasing flexibility up to 42%. Above 42%, the profit is not improved due to market conditions.

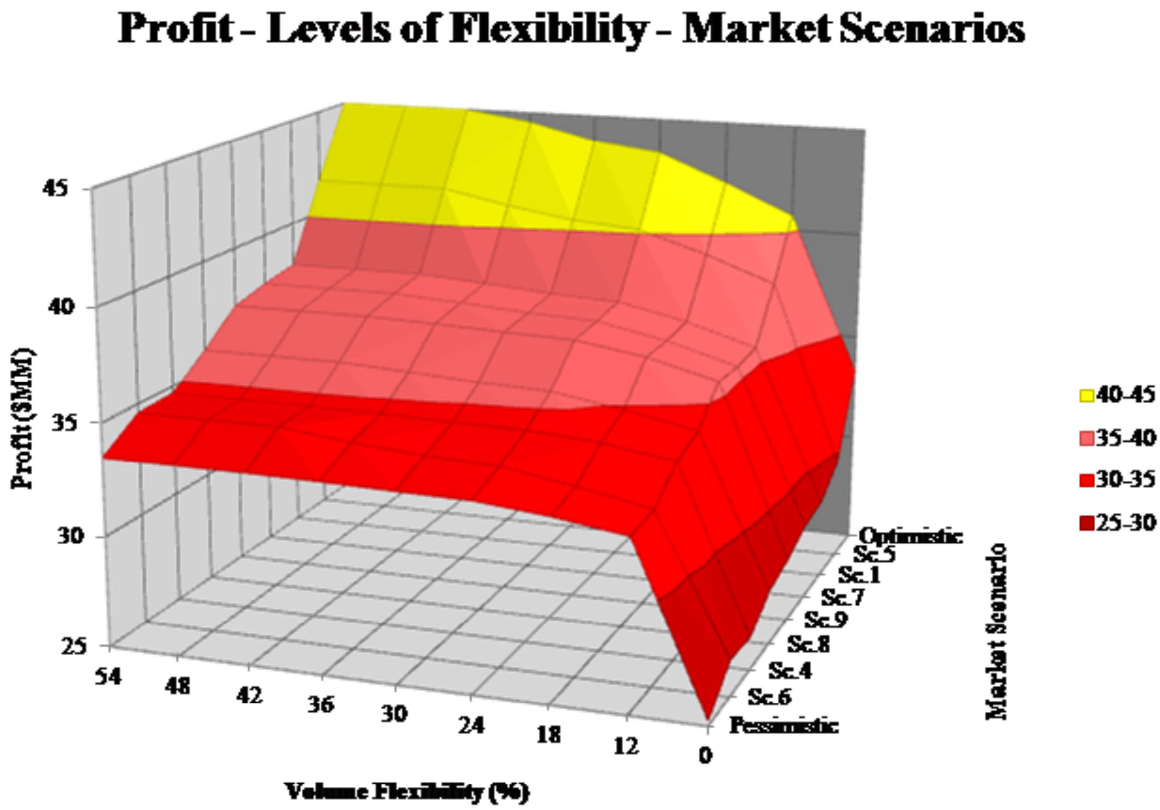


Figure 3-27 SC profit of each level of flexibility in case of market scenario realizations: B-1

Figure 3-28 illustrates the capital cost required for each flexibility level. From 0% to 30% volume flexibility, the increase in the capital cost is not significant, because with some slight modifications the level of flexibility can be improved. In order to go beyond this level, major modifications are required to be done on the process, which incur more cost. Moreover, with more flexibility, more capacity will be available and the capital cost required for the SC will grow. As a result, the capital cost increases more sharply after 30% volume flexibility. The result of profitability (ROI) analysis is shown in Figure 3-29. Up to 30% flexibility, the increase in capital cost can be compensated by the profit improvements. In flexibility levels higher than 30%, the capital cost rise plays the major role and profit improvement in this range is not enough to pay off the extra capital cost. Hence, 30% can be targeted as the optimum level of flexibility for this alternative.

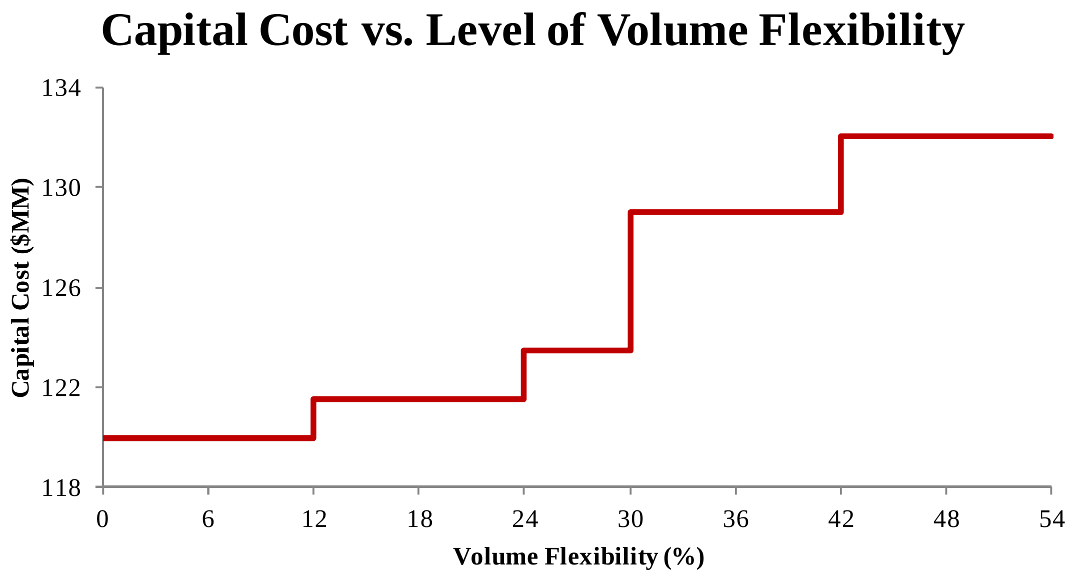


Figure 3-28 Capital cost for different levels of volume flexibility: B-1

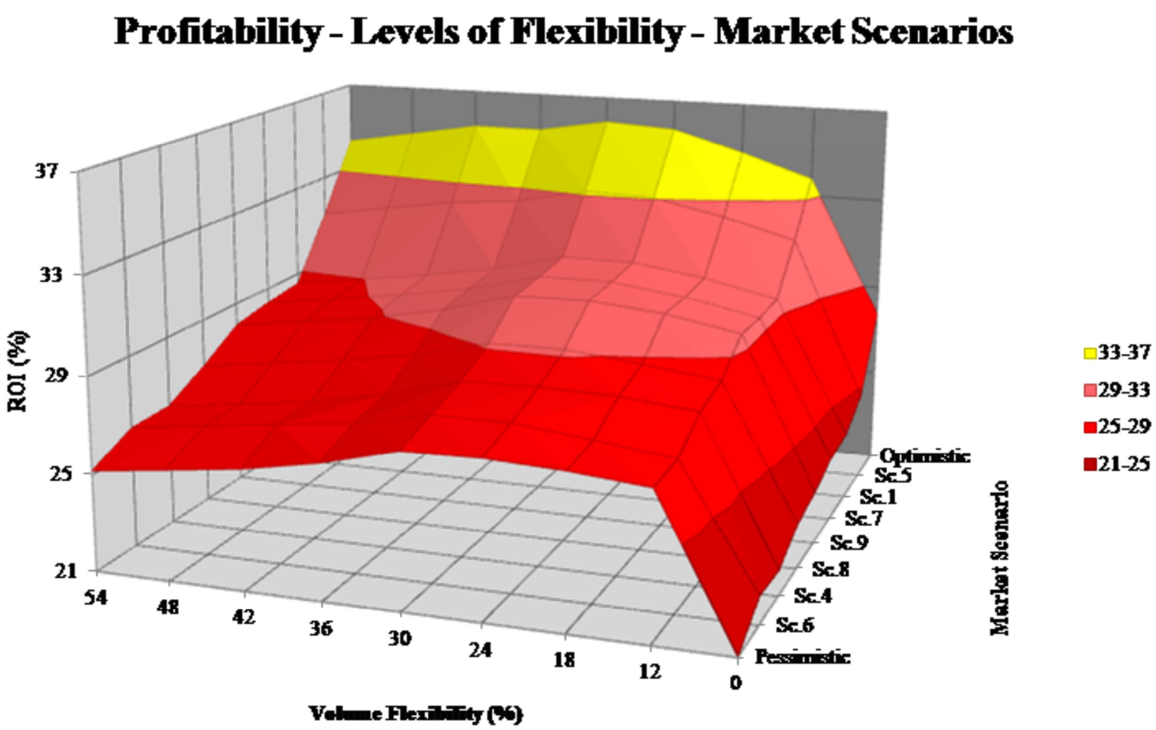


Figure 3-29 SC Profitability of each level of flexibility in case of market scenario realizations: Option B-1

Figure 3-30 illustrates the profit of all three thermochemical process alternatives for their own targeted flexibility. SC network alternatives associated with these process alternatives are those which exclude partnership in any stage, be it in processing level, in sales level, or in transportation level. The results for all combined alternatives will be presented and analyzed in the next section. It is observed that for all scenarios, the alternative with higher potential of flexibility has higher profit, though the profit improvement due to higher flexibility does not seem to be significant. Figure 3-31 depicts profitability, flexibility and robustness of each alternative. The value of MF shown in this graph is the average flexibility used by each alternative in all scenarios. Thus, in this case, MF doesn't show the overall flexibility of an alternative. As shown by MF in this figure, as the potential for flexibility increases, more flexibility is used. Moreover, as more flexibility is used, both profit (Figure 3-30) and robustness (Figure 3-31) increase, meaning that the SC is more robust against volatility. But profitability does not have the same behavior as flexibility increases. It is illustrated that alternative A-3, which has the highest potential for flexibility and also more flexibility is used on this alternative, has the lowest profitability. Again, that is due to the fact that profit improvement as a result of higher flexibility cannot compensate the increase in capital cost and the extra capital cost paid for more flexibility is not paid off in this case.

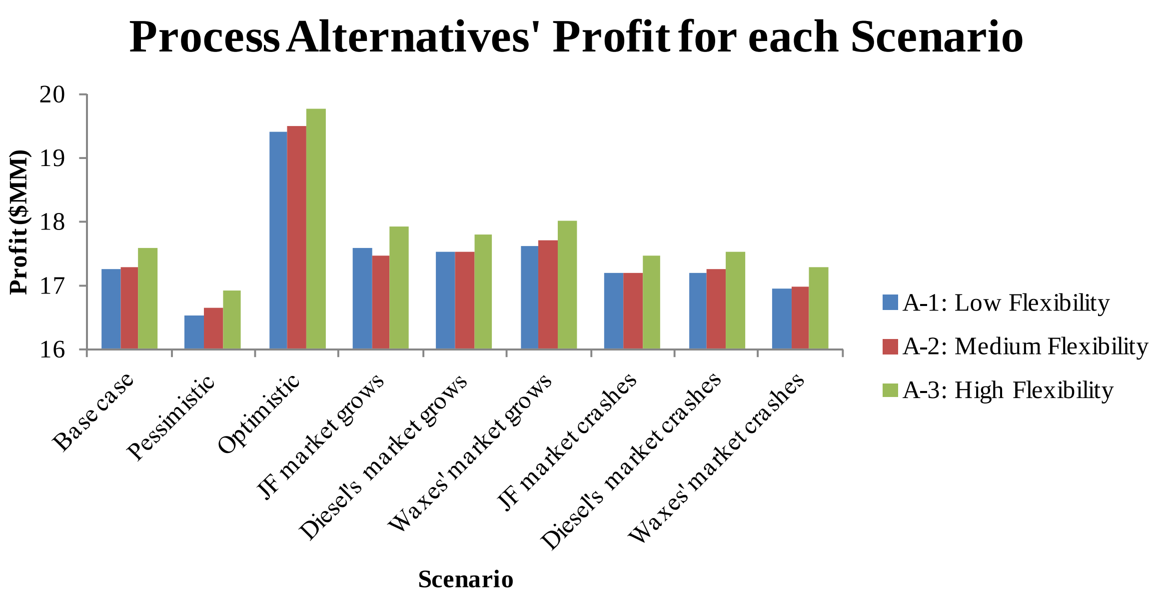


Figure 3-30 Profit of process alternatives for all scenarios: Thermochemical option

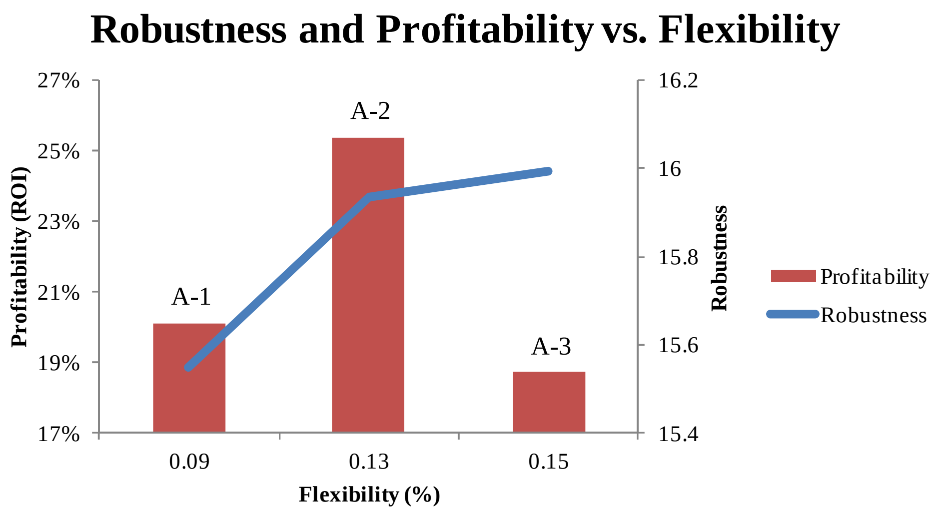


Figure 3-31 Robustness and profitability vs. flexibility: Thermochemical option

Same results are presented in Figure 3-32 and Figure 3-33 for the Biochemical option. Figure 3-32 shows the profit of two alternatives for their own targeted flexibility.

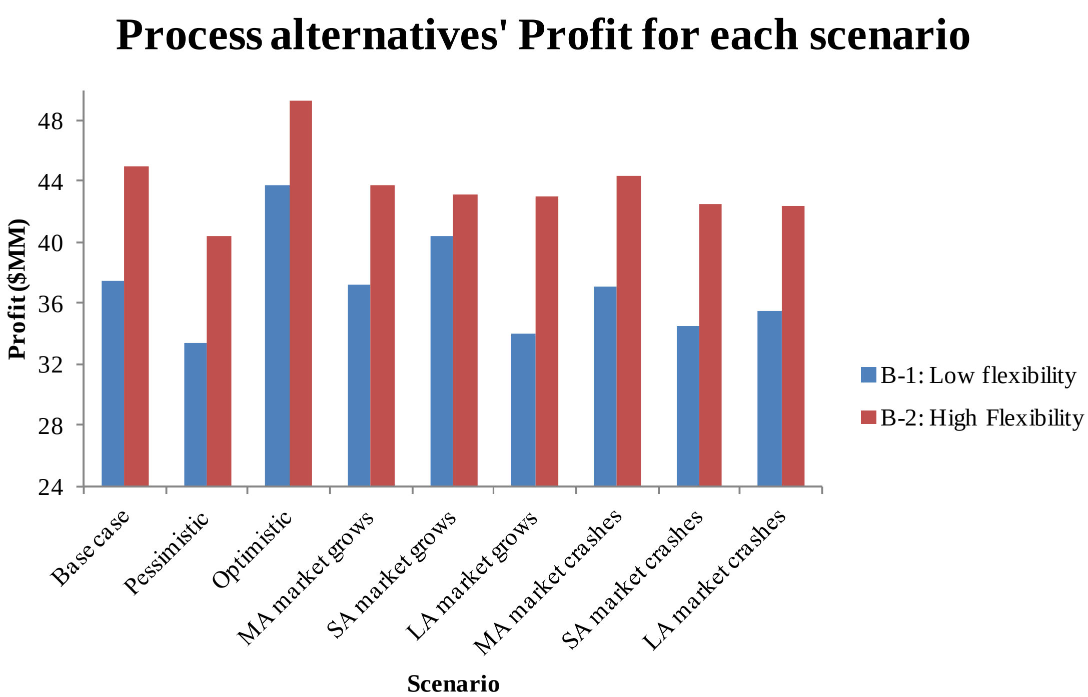


Figure 3-32 Profit of process alternatives for all scenarios: Biochemical option

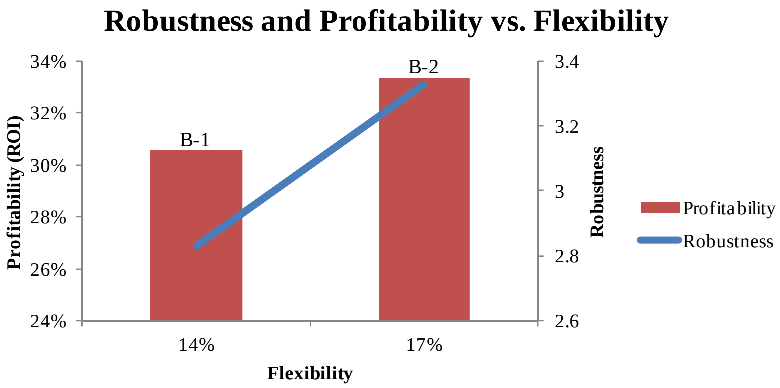


Figure 3-33 Robustness and profitability vs. flexibility: Biochemical option

It is clear that by increasing flexibility in this option, the profit is improved considerably. Figure 3-33 reveals that by increasing the potential for flexibility, more flexibility is used. Moreover, with more flexibility, profit (Figure 3-32) and robustness (Figure 3-33) are enhanced. Contrary to Thermochemical option, profitability also improves as flexibility increases. This means that for the Biochemical option, the extra capital cost paid for adding one recovery system for SA/MA to the first production line is very well compensated by the increase in capability of system to produce more profitable products.

In all, it can be seen that the first portfolio is more robust than the second portfolio, though the way market scenarios are defined has a direct effect on that. Furthermore, the first portfolio is not as sensitive as the second portfolio to volatility as the robustness doesn't change significantly from one case to another. But in second portfolio, the change in robustness is considerable.

3.3.3.1 Conclusion

Margins-based policy maximizes the entire SC profit by exploiting the system's flexibility so that the company is more robust against market volatility. Therefore, market volatility and all SC activities must be reflected in design of process flexibility. Results of this part demonstrate that:

- Flexibility is critical for a robust design and it improves the robustness of a system in response to market volatility.
- The cost of flexibility can be calculated and it can be illustrated that at what level of flexibility, having flexibility matters given the market volatility, i.e. the extra capital cost paid for having a higher level of flexibility is compensated by enhancing system's capability facing with market volatility.

- With the proposed approach, i.e. using SC analysis in targeting the flexibility, economic metrics can better be estimated. In the case of flexible processes that can produce several products in different production modes, the production sequence is not obvious. A deterministic sequence can be used, but as shown by the results, a deterministic sequence cannot result in the highest profit. In fact, calculating the profit of a flexible production system without a SC analysis is impossible due to the ambiguity of the production sequence. A SC analysis can determine the optimum production sequence and calculate the associated profit.

3.3.4 Designing the supply chain network

The results for each combined alternative are presented in this section. Process alternative A-1 has two SC network alternatives at the processing level, one implying sending diesel to a JF producer and one including JF production at the mill. The IRR and robustness of these two combined alternatives are illustrated in Figure 3-34. The IRR of the option of sending diesel to JF producer is much higher than that of producing JF at the mill. It means that producing JF at the mill, with current price or production cost, is not profitable. Therefore, company may sell its diesel to a JF producer which will also secure company's diesel market. But, it can be seen that the robustness of the option of producing JF at the mill is higher. That is because of the increase in flexibility. The system is more flexible when it produces one more product. It gives more flexibility to the company in a volatile market, and thus makes it more robust against market volatility.

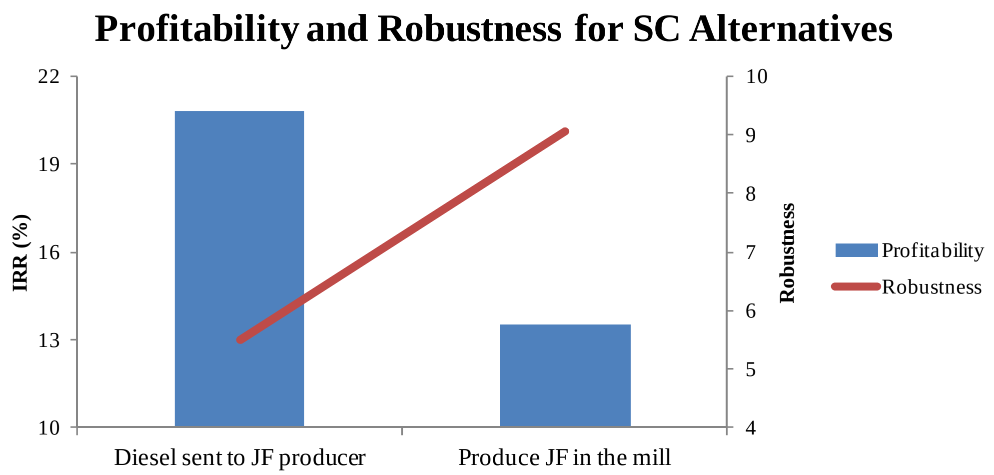


Figure 3-34 Profitability and Robustness for SC Alternatives: A-1

Process alternative A-2 has two SC network alternatives at the sales level; sending diesel to a partner or selling it on the spot. Figure 3-35 reveals that both alternatives have almost equal IRR, but robustness of sending diesel to a partner is higher. The reason is that in this way the company externalizes the risk of facing with volatility in diesel market by transferring it to the partner.

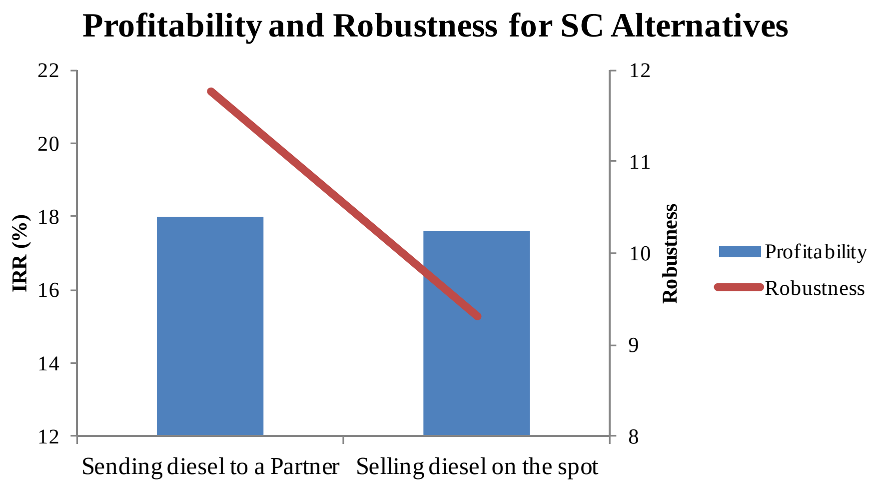


Figure 3-35 Profitability and Robustness for SC Alternatives: A-2

Process alternative A-3 is associated with two SC network alternatives at the transportation level; buying trucks, i.e. own fleeting, or making contract with a transportation company. Figure 3-36 shows that both alternatives have almost equal IRR and robustness. However, although from an economic point of view there is no difference between these two alternatives, second alternative implies less risk and responsibility. Instead of buying a network of trucks and taking care of them and their logistics, the company can easily outsource its transportation system and still have the same economic result.

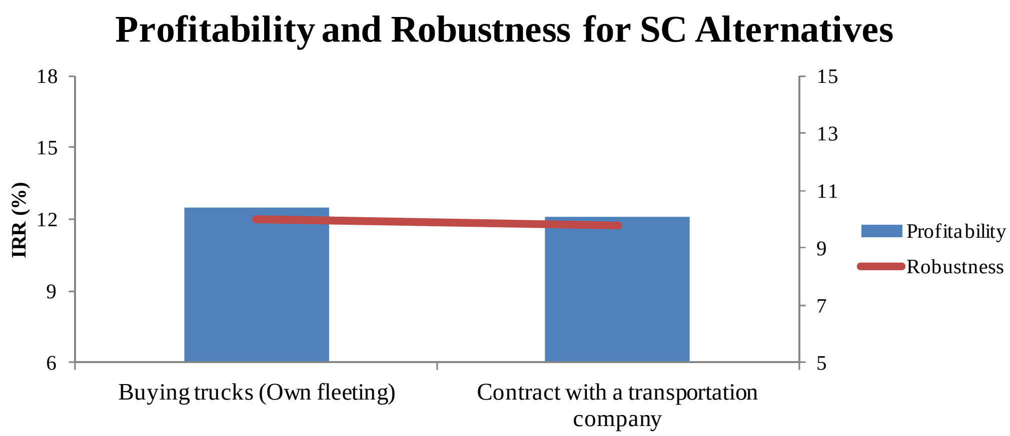


Figure 3-36 Profitability and Robustness for SC Alternatives: A-3

The process alternatives of Biochemical option have two SC network alternatives at the processing level; either sending the extractives to a partner or processing them at the mill. Unlike the Thermochemical option for which producing JF at the mill is less profitable than sending it to a JF producer, for the Biochemical option processing the extractives at mill is much more profitable than sending it to a partner, as illustrated in Figure 3-37. This is due to the fact that extractives being processed at the mill are used to produce xylitol, which is a very high-value product. The results approve that added-value products can significantly increase the profitability of a company compared to commodities. The high profit associated with added-value chemicals helps them internalize the risk of volatility, i.e. the profit may decrease due to market volatility, but remains still high compared to commodities. In addition, robustness of the alternatives which involve processing the extractives at the mill is considerably higher than the robustness of alternatives which include sending the extractives to a partner. This again supports the notion that robustness improves with flexibility. The flexibility of the system is higher in the case the extractives are processed at the mill, because of producing one more product.

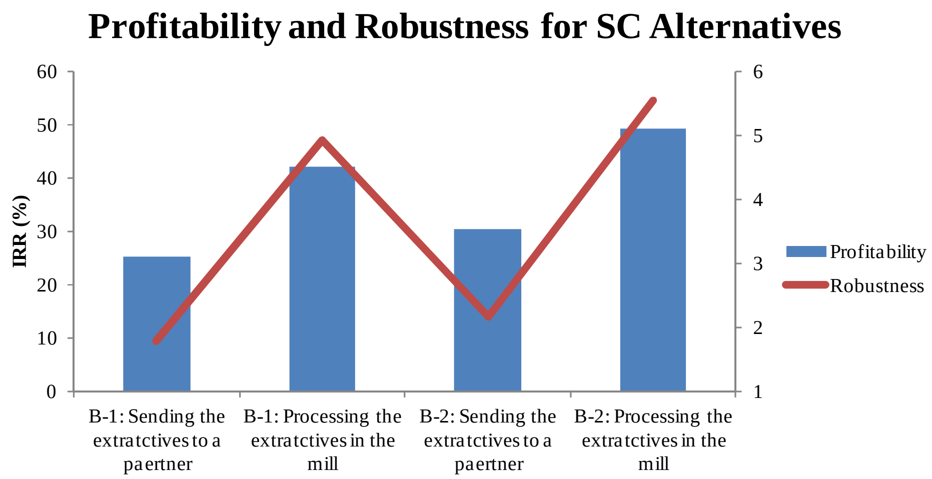


Figure 3-37 Profitability and Robustness for SC Alternatives: Biochemical option

An important point to be mentioned is that the design of a process alternative affects the design of SC network alternatives and the strategies of SC management at the operational level. Figure 3-38 and Figure 3-39 illustrate that, in similar market conditions, different patterns of order acceptance is chosen for different levels of flexibility, i.e. for option B-1 and option B-2, which might imply different inventory management, different sales strategies, and different transportation strategies. Therefore, there is a direct link between process design and SC network design and it is worth integrating them.

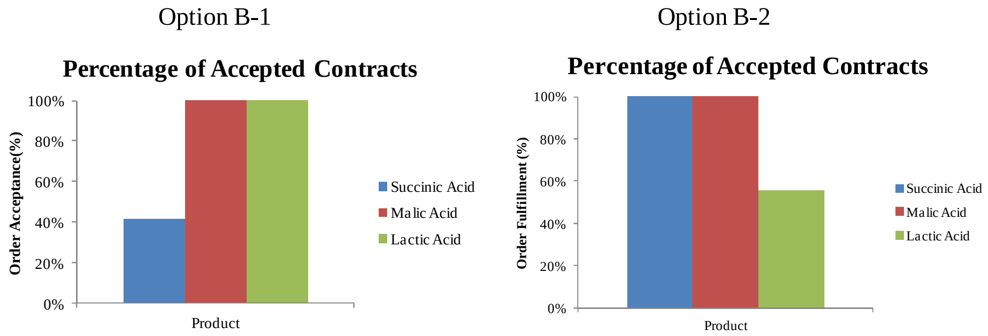


Figure 3-38 Percentage of accepted contracts: Biochemical options

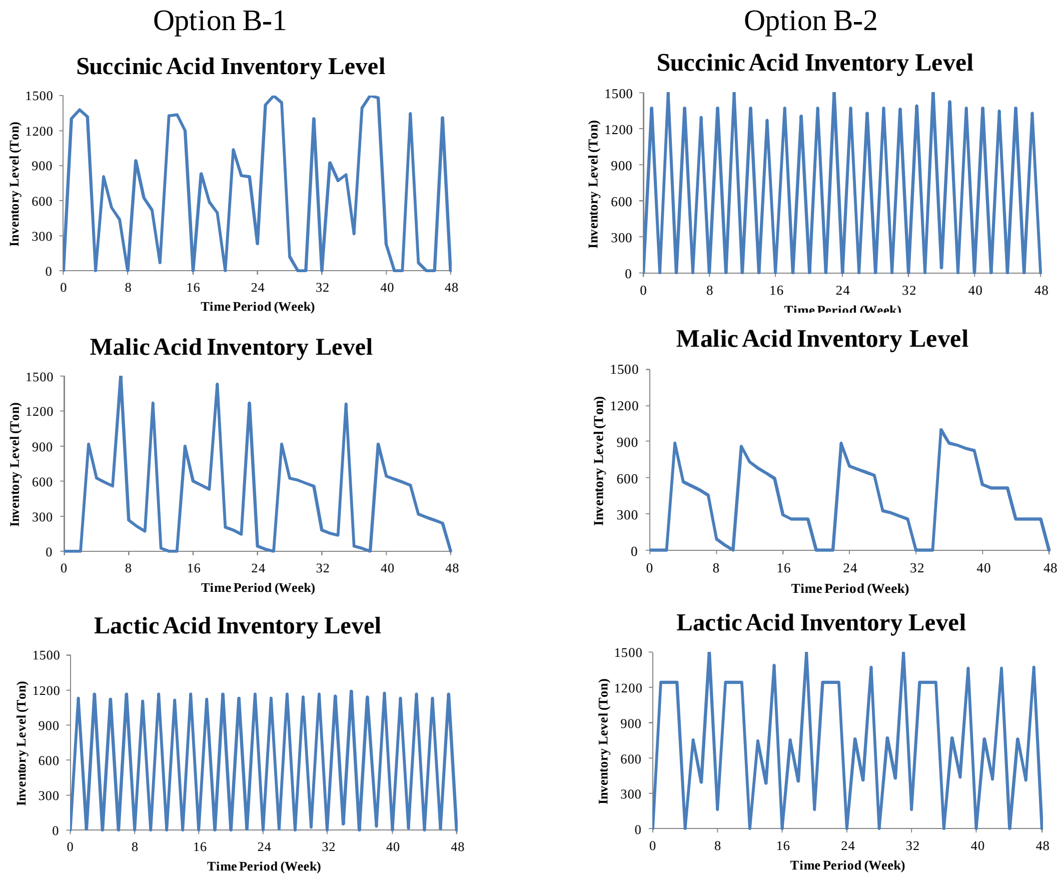


Figure 3-39 Inventory levels: Biochemical options

3.3.4.1 Conclusion

There is a need for an approach which considers the constraints a company deals with in reality, and given these constraints, makes a direct link between possible process and SC network alternatives to propose practical solutions. With the proposed approach, i.e. defining SC alternatives related to process alternatives, the following aspects can be addressed related to process alternatives:

- As a result of change in level of flexibility and thus, change in production capacity, the procurement, transportation, and selling costs and strategies will be different. Only a SC analysis can takes into account all these changes.
- The inventory levels and storage capacity will also be different for different levels of flexibility. Again, a SC analysis can calculate the inventory level of each product according to the production sequence and determine the storage capacity required for each product.
- The possible SC options for a company can be identified and their performance at the operational level can be evaluated

3.3.5 Phased approach for implementing biorefineries

For each option, three strategies were defined after discussion with mill's executive board. Each strategy is implemented through one or more than one phases. These strategies are introduced in Figure 3-40 and Figure 3-41. Strategy I for Thermochemical option includes one phase in which the FTL process is implemented. Strategy II involves two phases; in the first phase the FTL process is implemented and then in the second phase a hydro-treating process is added to convert the whole diesel to JF. Strategy III is implemented in three phases; FTL process is implemented first, then a hydro-treating process is added to convert half of diesel to JF and finally, another hydro-treating process is added so that the whole diesel can be converted to JF.

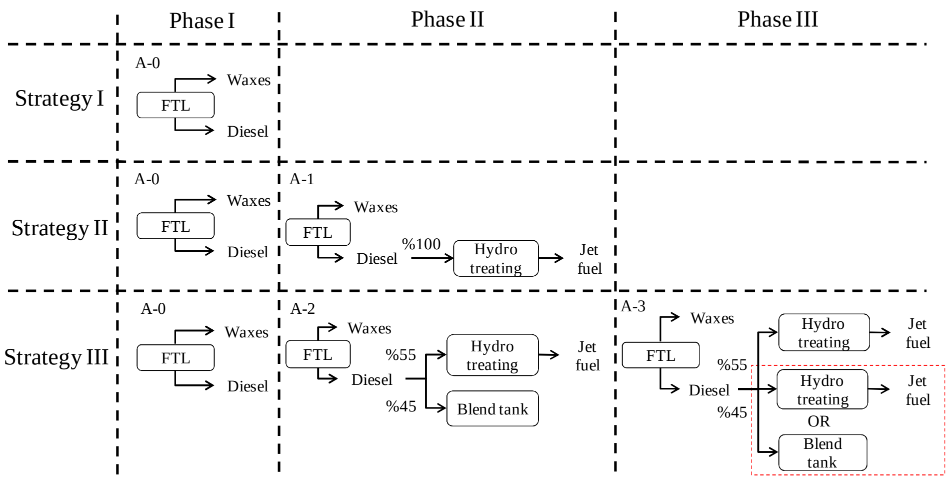


Figure 3-40 Phased implementation strategies: Thermochemical option

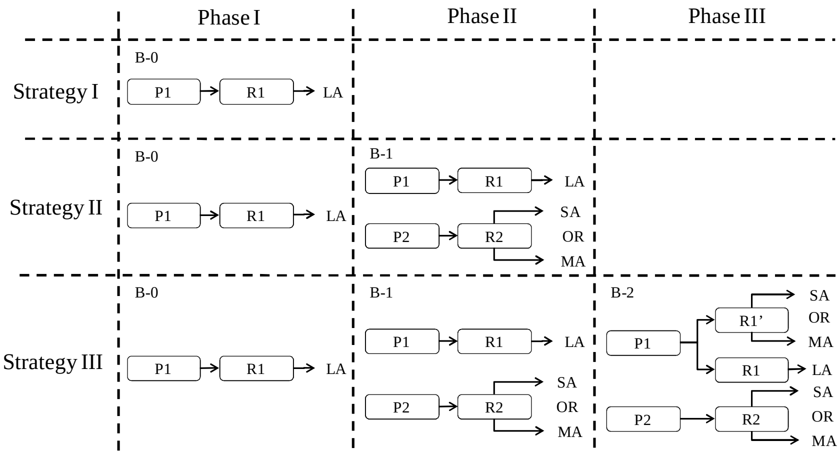


Figure 3-41 Phased implementation strategies: Biochemical option

Strategy I for Biochemical option consists of one phase in which one line for producing LA is installed. Strategy II comprises of two phases; in the first phase LA production line is installed and in the second phase, the second line for producing SA and MA is added. Strategy III is done within three phase; in the first phase LA line is installed, then second line will be added to produce SA and MA, and finally an extra recovery system for SA and MA will be added to the first line to make it capable of producing all three acids.

3.3.5.1 Thermochemical option

The profitability analysis was performed for nine major scenarios made to represent market volatility. A Monte Carlo simulation was also carried out to take into account more random changes in the uncertain market parameters. The assumptions for the profitability analysis are summarized in Table 3-9.

Table 3-9 Assumption for profitability analysis: Thermochemical option

Item	Description
Depreciation	Linear over 20 years
Tax	10%
Project start date	2013 70% of total capital spending
Duration of construction	2 years
Capital cost expenditure	50% each year
Phase II implementation	In the 5th year after start-up 15% of total capital spending
Phase III implementation	In the 9th year after start-up 15% of total capital spending
Price change	2% every year

The result of profitability analysis is presented in Figure 3-42

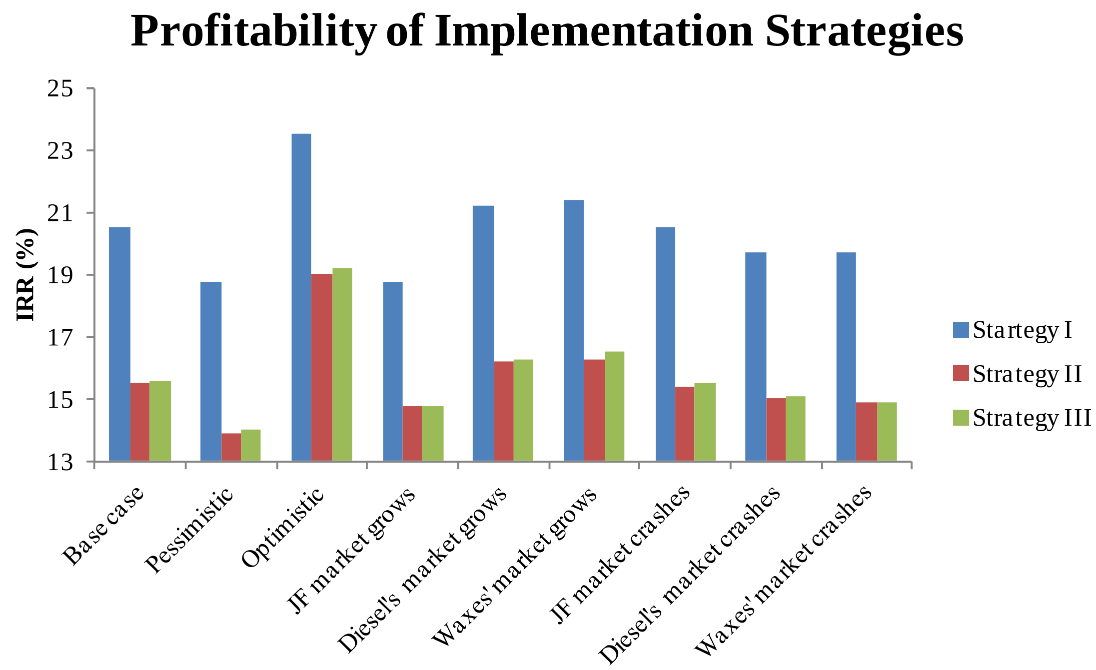


Figure 3-42 Profitability of Implementation Strategies: Thermochemical option

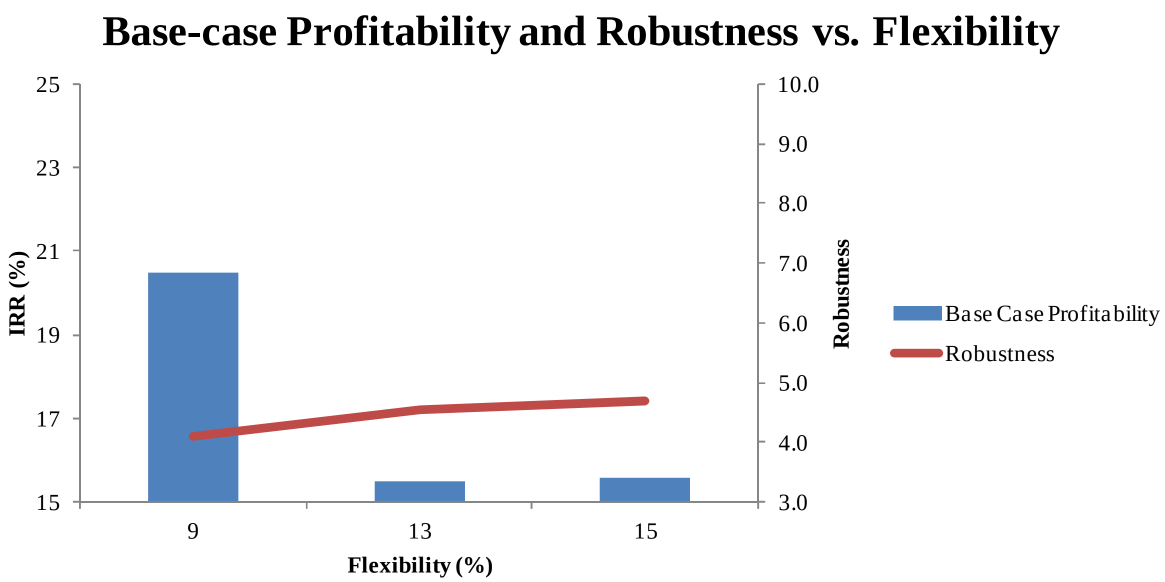


Figure 3-43 Base-case Profitability and Robustness vs. Flexibility: Thermochemical option

It is seen that the IRR of strategy I is much higher than that of two other strategies. It implies that producing JF with the current price and/or production cost is not profitable. Strategy III is a bit more profitable than strategy II in most of scenarios, but the difference is not significant at all. Figure 3-43 shows that although the profitability of strategy I is higher, its robustness is slightly lower than that of other's, which is due to having lower flexibility compared to others.

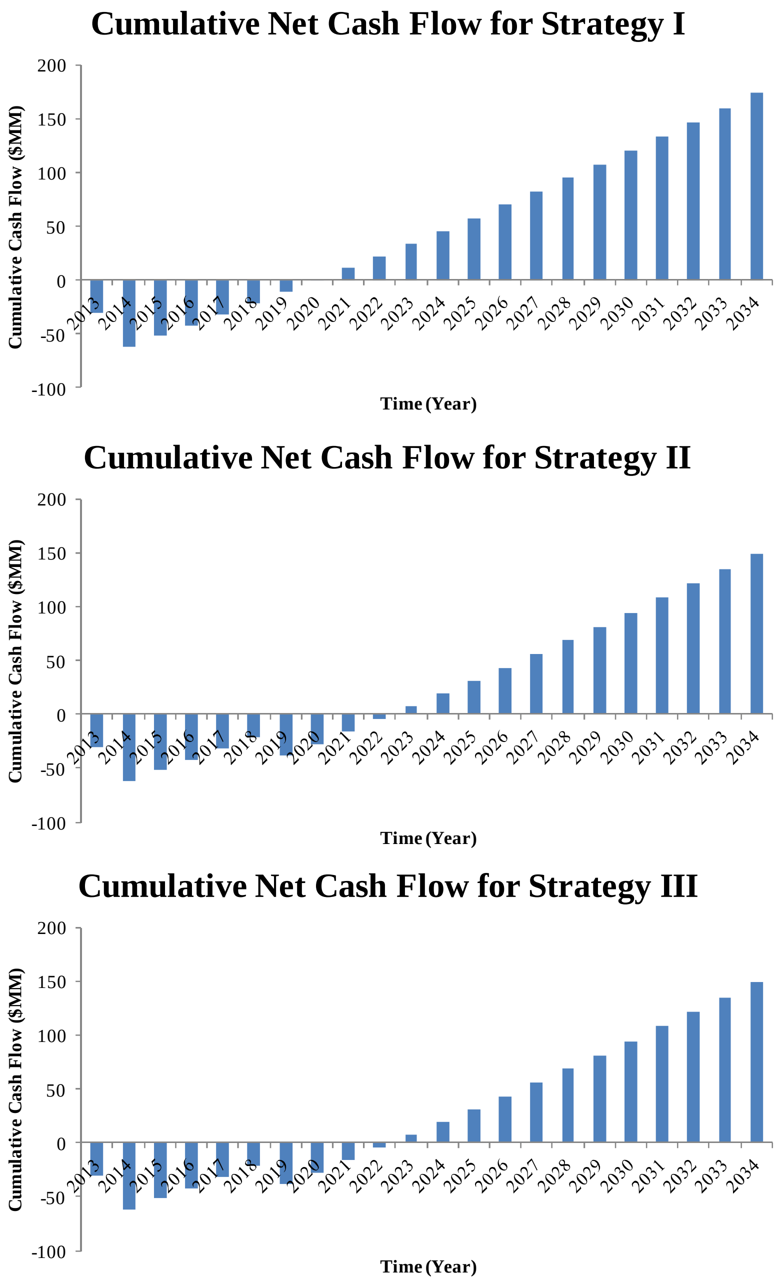


Figure 3-44 Cumulative net cash flow for strategies: Thermochemical option

Figure 3-44 illustrates the cumulative net cash flow (CCF) of each strategy. It can be seen that strategy I has the highest CCF.

A number of sensitivity analyses were carried out to identify the sensitivity of each strategy to change in critical parameters. Figure 3-45 reveals the sensitivity of downside IRR (related to the pessimistic scenario) to feedstock and electricity price. First of all, the sensitivity of strategy II and strategy III in both cases are similar. All strategies are not very sensitive to electricity price, but very sensitive to feedstock price. By a $15/ton increase in feedstock price, the IRR for the first strategy enters a range which makes the project non-profitable. This happens for strategy II and strategy III by only $10/ton increase in price.

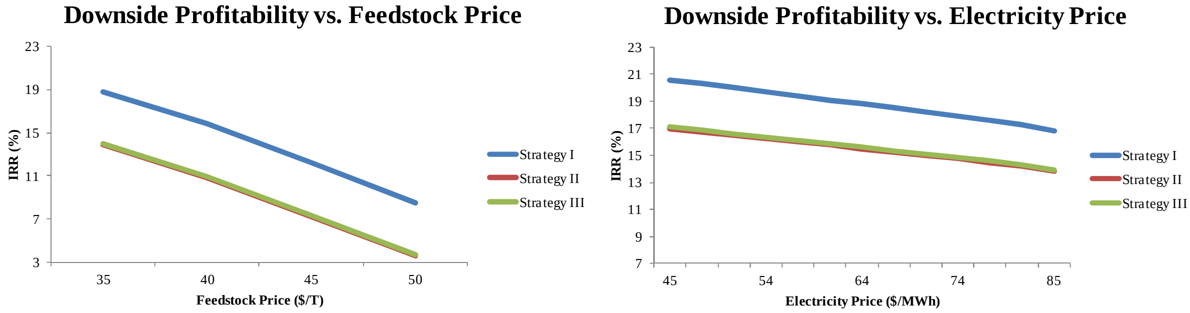


Figure 3-45 Sensitivity analysis on feedstock and electricity price: Thermochemical option

Figure 3-46 shows the sensitivity of IRR to product price for strategy I. On the left, it is observed that the IRR drops with a sharp slope as product prices decrease. By $1/Gal decrease, the IRR will be under 10%. On the right, the sensitivity to aggregate decrease in all product prices is plotted. 20% decrease in all product prices reduces the IRR to almost zero.

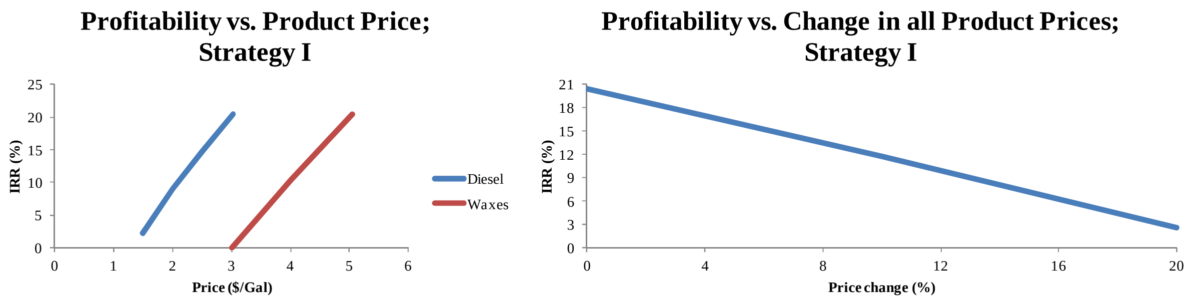


Figure 3-46 Sensitivity analysis on product price: Thermochemical option (Strategy I)

Figure 3-47 shows the same analysis for strategy II. The IRR sensitivity to wax price is the same as strategy I. As the production level of diesel is smaller compared to strategy I, this strategy is less sensitive to diesel price. Moreover, as the system is flexible and can lower the production of

JF or stop its production when JF price decreases to a certain value, the system will shift to diesel. Thus, the IRR won't change after that value. If this flexibility had not existed, the IRR would have followed the dashed line. The same analysis was done for the production cost of each product. Figure 3-48 illustrates this analysis for strategy III. Again, flexibility in diesel and JF production helps to maintain the IRR high when the price of one of them decreases.

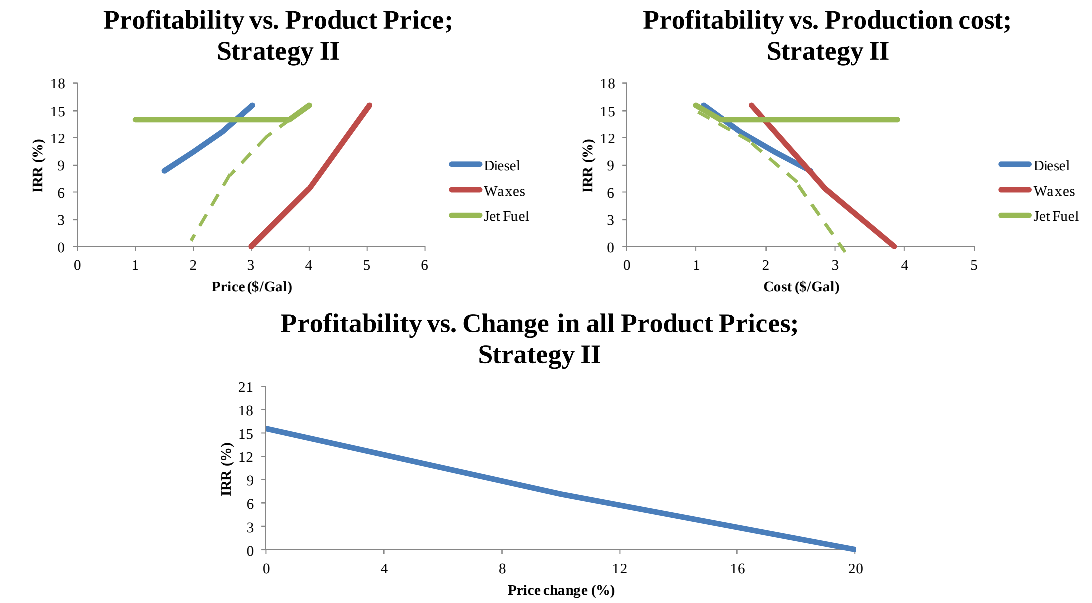


Figure 3-47 Sensitivity analysis on product price: Thermochemical option: Strategy II

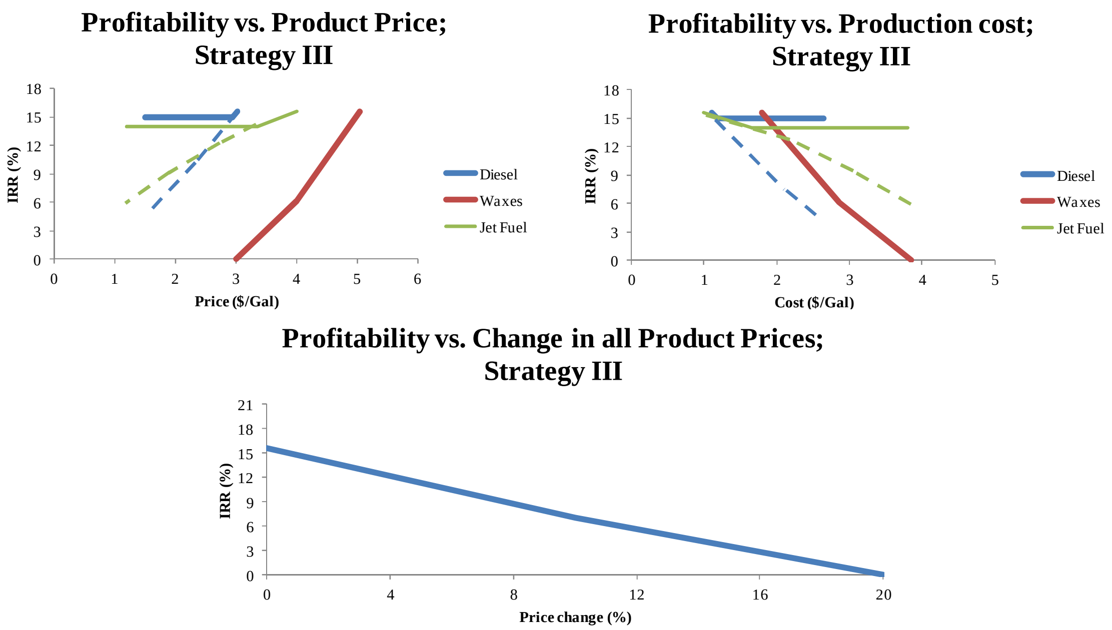


Figure 3-48 Sensitivity analysis on product price: Thermochemical option: Strategy III

Figure 3-49 shows what the JF price should be to make strategy II and strategy III as profitable as strategy I. JF price must be \$1.4/Gal higher for the strategy II to be as profitable as strategy I does. This price difference must be \$2.4/Gal for strategy III.

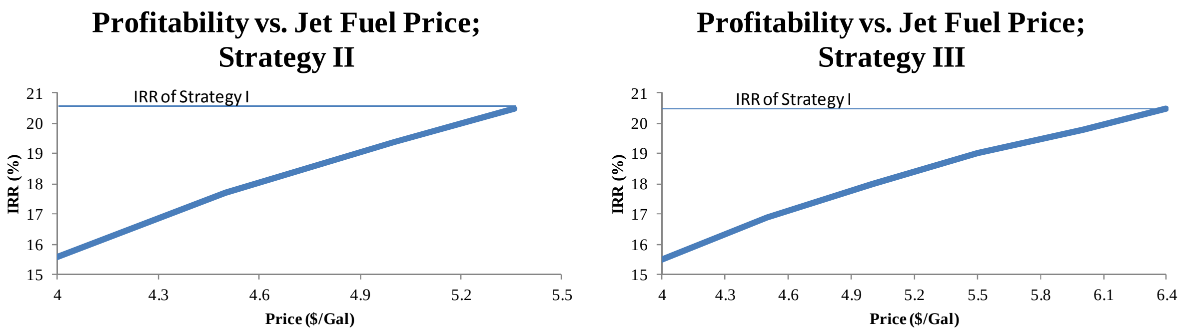


Figure 3-49 IRR of strategies II and III vs. JF price

Lastly, a Monte Carlo analysis was done on feedstock price and product prices. The price distributions are presented in Figure 3-50. The results are shown in Table 3-10 and Figure 3-51. Strategy I has the highest profitability and the highest standard deviation in IRR, thus the lowest robustness among other strategies. This is due to the fact that strategy I has the lowest potential for flexibility compared to other strategies.

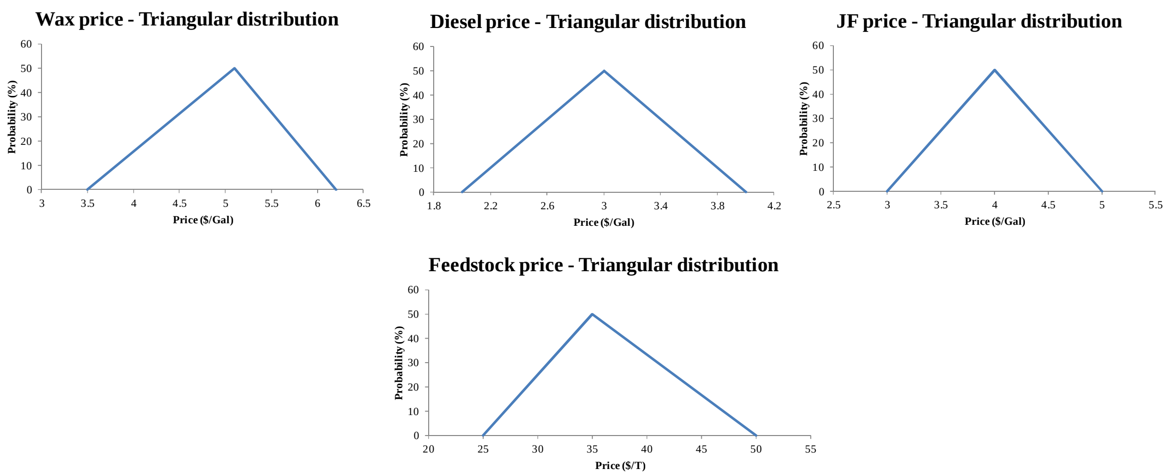


Figure 3-50 Price probability distributions: Thermochemical option

Table 3-10 Result of Monte Carlo simulation: Thermochemical option

Strategy	IRR (%)	Standard deviation (%)
Strategy I	20.4	7.24
Strategy II	15.5	6.1
Strategy III	15.6	6.2

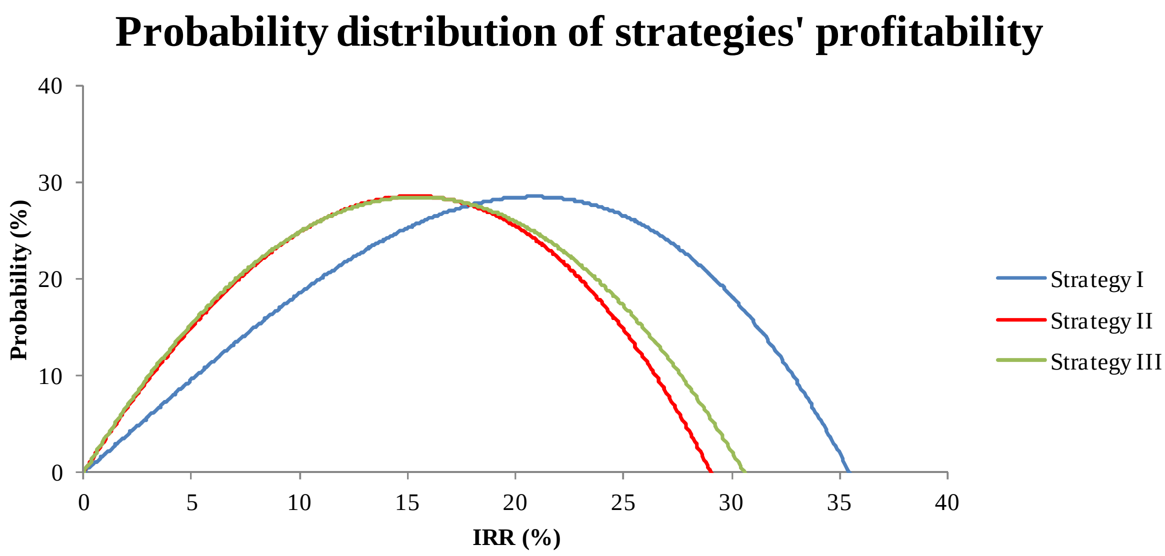


Figure 3-51 Probability distributions of IRR: Thermochemical option

3.3.5.2 Biochemical option

The assumptions for the profitability analysis are summarized in Table 3-11.

Table 3-11 Assumption for profitability analysis: Biochemical option

Item	Description
Depreciation	Linear over 20 years
Tax	10%
Project start date	2013 45% of total capital spending
Duration of construction	2 years
Capital cost expenditure	50% each year
Phase II implementation	In the 5th year after start-up (taking 2 years) 47% of total capital spending
Phase III implementation	In the 9th year after start-up (taking 1 year) 8% of total capital spending
Price change	2% every year

The result of profitability analysis for nine major market scenarios is presented in Figure 3-52. The IRR of strategy II and strategy III are much higher than that of strategy I. It implies that producing more value-added products such as SA and MA improves the profitability of the strategies. The IRR of Strategy III is also higher than that of strategy II in all scenarios, which denotes that increasing flexibility will have a positive effect on the profitability for this option and the extra capital cost will be compensated. Figure 3-53 affirms that, for the Biochemical option, both profitability and robustness improve by increasing flexibility. Figure 3-54 presents the CCF of each strategy. Strategy I has a much lower CCF compared to second and third strategies, though it has a two-year shorter payback period.

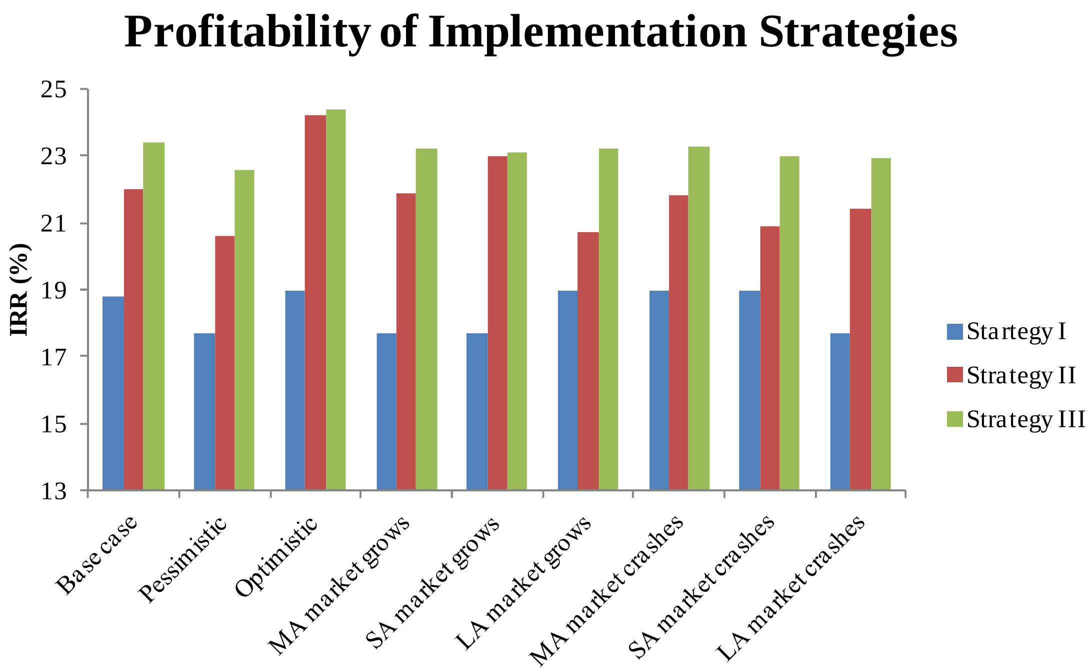


Figure 3-52 Profitability of Implementation Strategies: Biochemical option

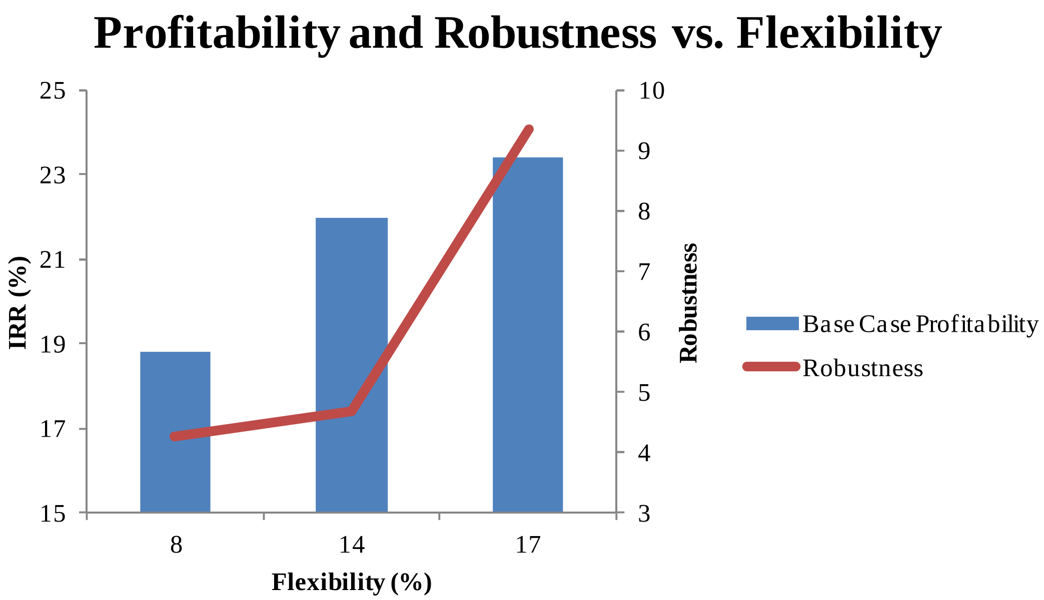


Figure 3-53 Base-case Profitability and Robustness vs. Flexibility: Biochemical option

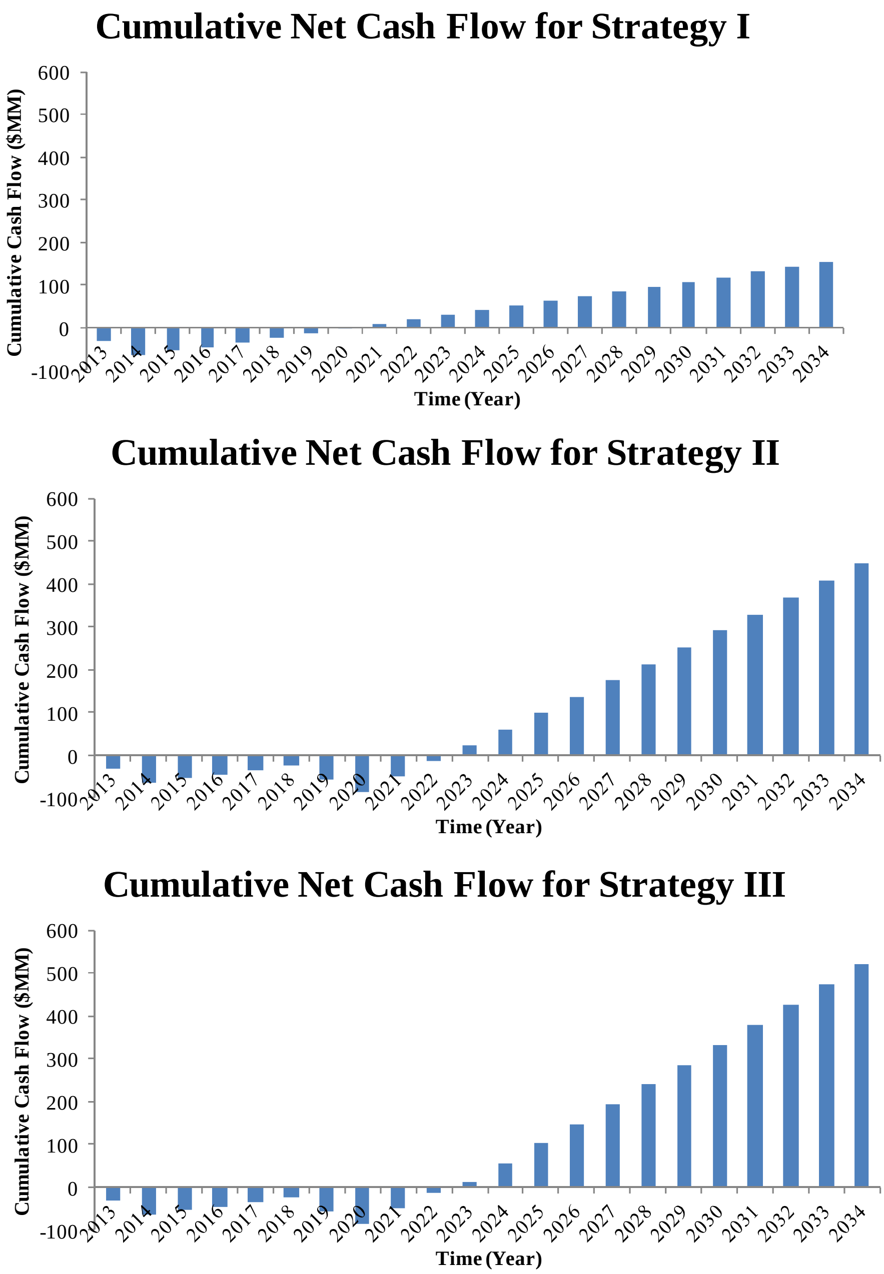


Figure 3-54 Cumulative net cash flow for strategies: Biochemical option

Figure 3-55 illustrates the sensitivity of downside IRR on product and fuel price. Compared to Thermochemical option, the difference between strategies in Biochemical option in terms of their sensitivity is tremendous. Strategy I can cope with feedstock price increase up to $15/Ton, while this amount for strategy II and strategy III is $30/Ton and $35/Ton, respectively. The same trend can be seen for sensitivity on fuel price. An increase of $150/Ton in fuel price pushes strategy I into the range of low profitability, while $250/Ton and $300/Ton increase in fuel price would have the same outcome for strategy II and strategy III, respectively.

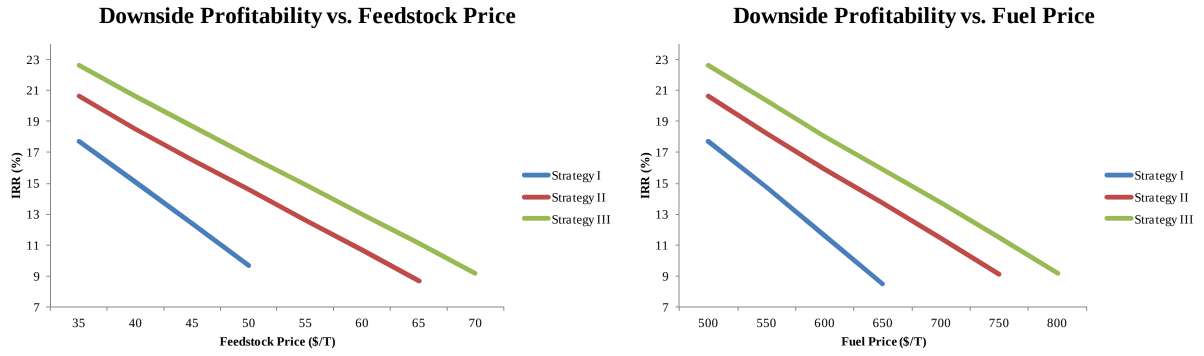


Figure 3-55 Sensitivity analysis on feedstock and fuel price: Biochemical option

Sensitivity of IRR on product price for strategy I is depicted in Figure 3-56. As can be seen, the IRR is quite sensitive to LA price and a decrease of $150/Ton in price makes the project non-profitable.

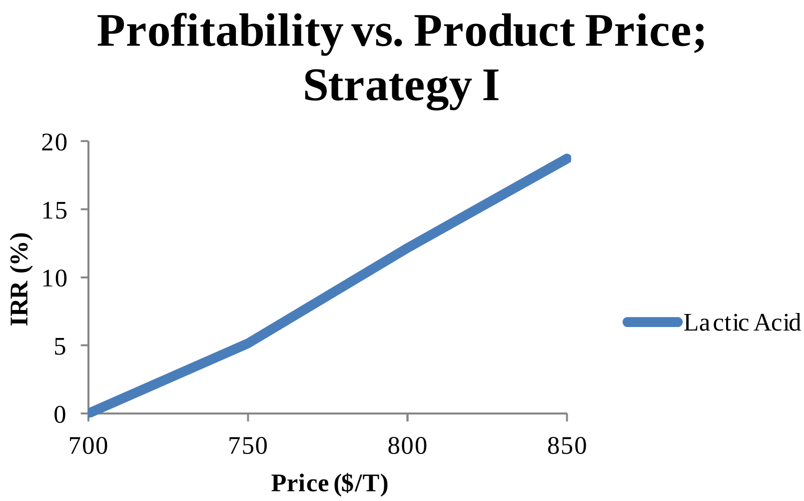


Figure 3-56 Sensitivity analysis on product price: Biochemical option (Strategy I)

Figure 3-57 shows the same analysis for strategy II. It can be seen that with $350/Ton decrease in LA price, the same IRR drop as what was seen in strategy I happens. That is because, in this case, there are other sources of income for company, i.e. from SA and MA. It can also be elicited that the system is sensitive to MA price, but as this product is extremely added-value, if its price drops to a value almost equal to its production cost, project still has an acceptable IRR. Sensitivity to SA price is also high, but again, even with 100% decrease in SA price, the project is still in the range of acceptable profitability. Same analysis was carried out for the production cost. With huge increases in SA and MA production cost, the project is still profitable, whereas LA production cost increase drops the IRR dramatically. Sensitivity of IRR to price decrease for all products are also shown in this figure.

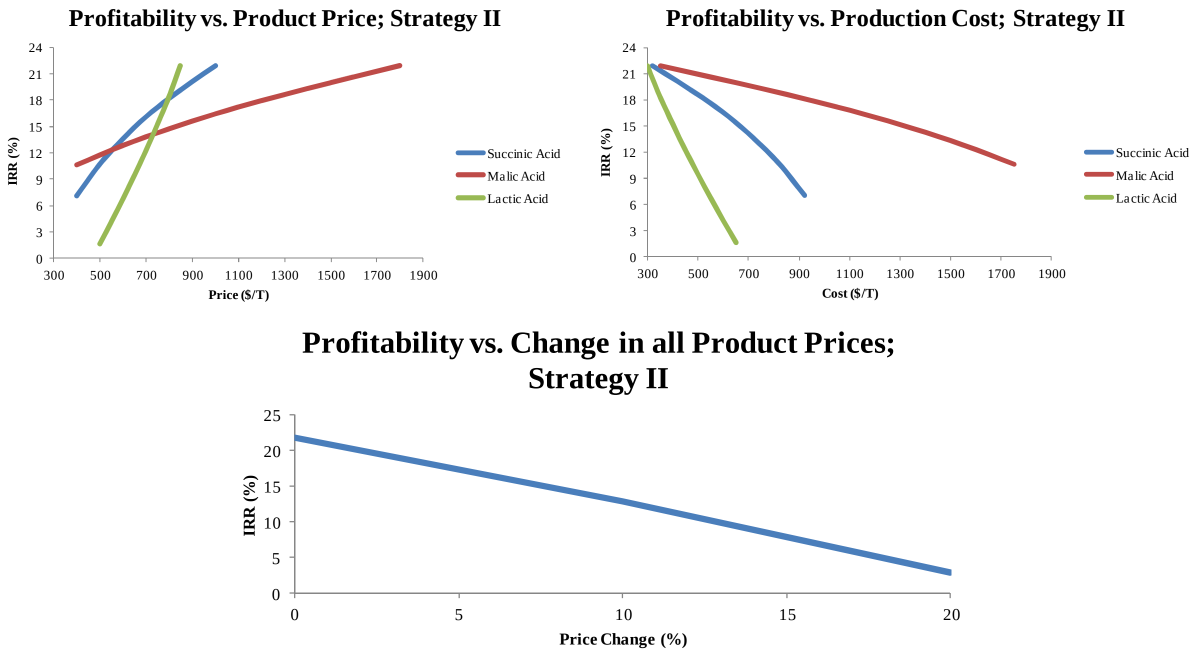


Figure 3-57 Sensitivity analysis on product price: Biochemical option (Strategy II)

The result of sensitivity analysis on the product price and production cost for strategy III, shown in Figure 3-58, reveals that the system's reaction to LA price decrease improves due to the fact that, in this alternative, the first production line is also able to produce SA and MA, and less LA is produced. Because of the same reason, the system gets more sensitive to SA price. The effect of increasing flexibility can also be seen in the sensitivity to production cost increase. Because of high margins associated with SA and MA, the system is not very sensitive to their production cost. Furthermore, increasing flexibility lowers the system's sensitivity to LA production cost increase. This is all the result of the fact that in third strategy LA has a smaller role in the profitability of the entire system compared to first and second strategies.

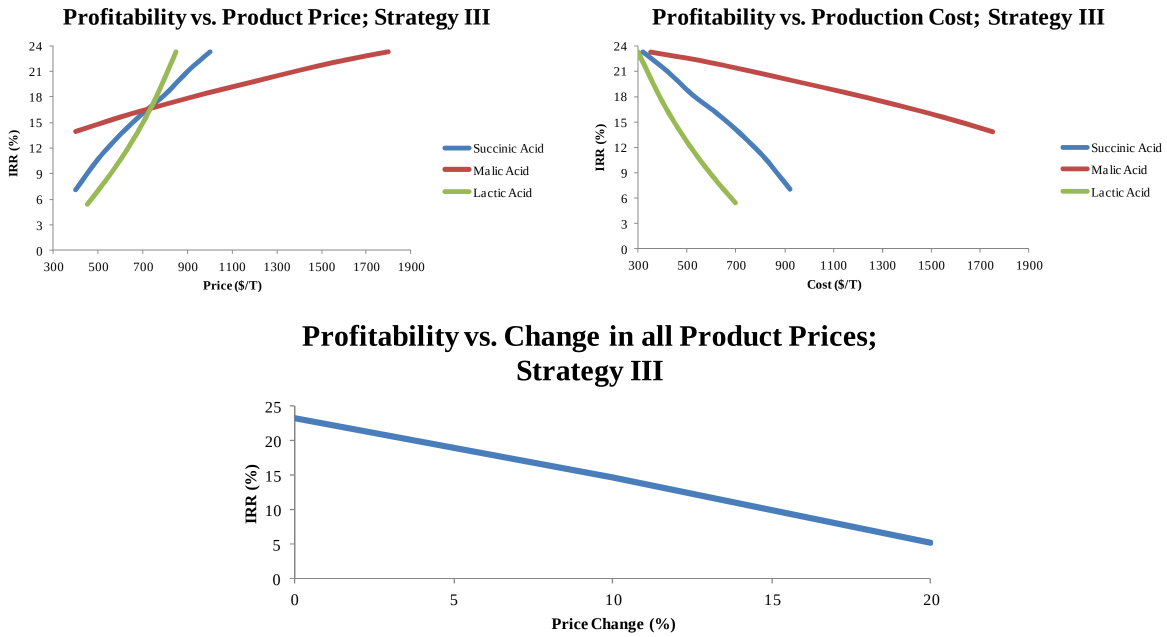


Figure 3-58 Sensitivity analysis on product price: Biochemical option (Strategy III)

A Monte Carlo analysis was done on feedstock price and product prices. The price distributions are presented in Figure 3-59. The results are shown in Table 3-12 and Figure 3-60.

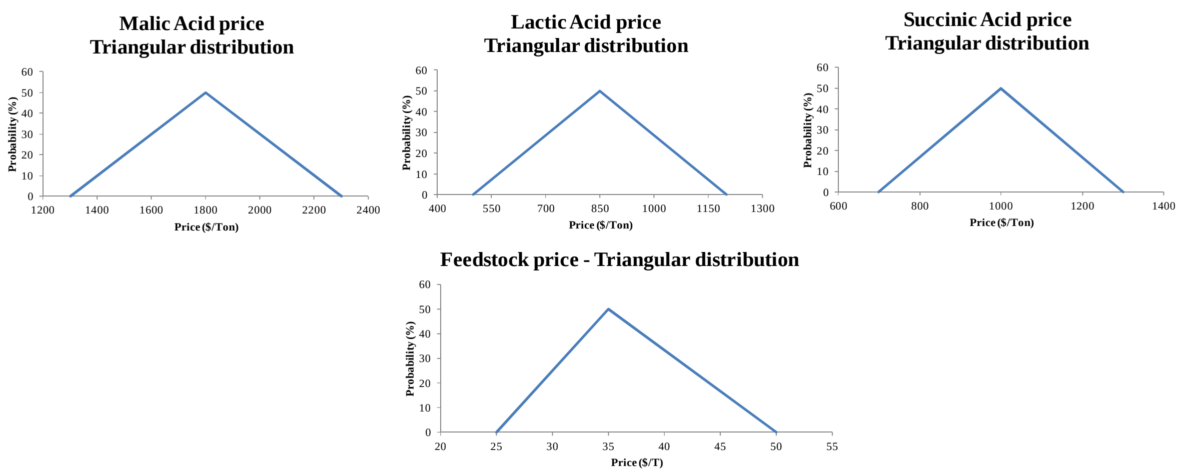


Figure 3-59 Price probability distributions: Biochemical option

Table 3-12 Result of Monte Carlo simulation: Biochemical option

Strategy	IRR (%)	Standard deviation (%)
Strategy I	18.8	13.9
Strategy II	21.9	9.3
Strategy III	23.3	8.9

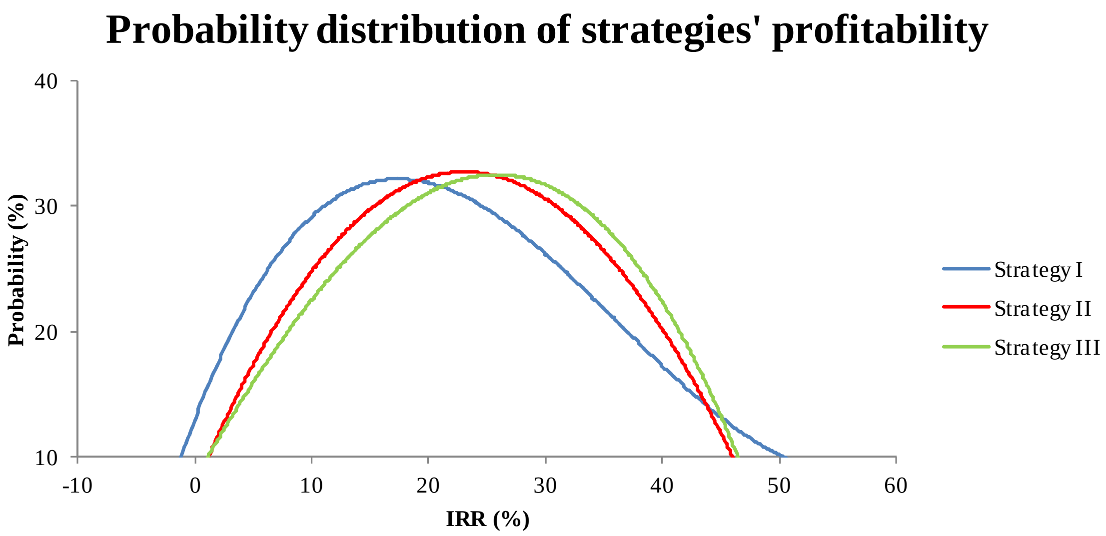


Figure 3-60 Probability distributions of IRR: Biochemical option

The result of Monte Carlo simulation is consistent with the results presented before. The profitability of strategy III is the highest. Moreover, the standard deviation of the calculated IRRs for this strategy has the smallest value, which connotes that strategy III is the most robust strategy among others. This supports the claim that when flexibility increases, the robustness of the system improves.

Lastly, the sensitivity of the system to the aspects related to process integration was studied. Figure 3-61 demonstrates that IRR is quite sensitive to the percentage of extracted hemicelluloses. The reason is that the extracted percentage is directly related to xylitol production yield. Xylitol is highly value-added and comprises around 25% of net revenue. Figure 3-62 shows how sensitive the IRR is to percentage of lignin separation. Separated lignin is used as fuel. Thus, decreasing the yield of lignin separation results in increasing the amount of fuel required for energy production.

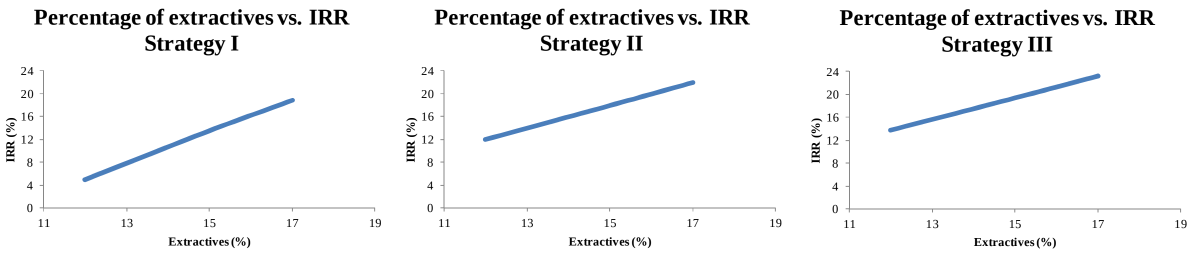


Figure 3-61 Sensitivity to extractives percentage

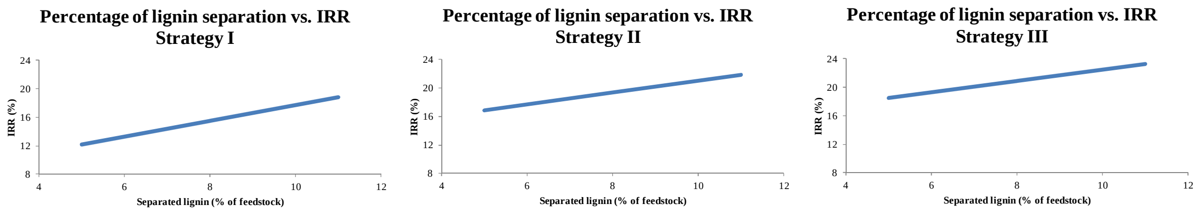


Figure 3-62 Sensitivity to lignin separation

3.3.5.3 Conclusion

The result of phased implementation analysis shows that proposed strategies for Thermochemical option to make it more flexible over the long term are less profitable than the strategy which implements the least flexible configuration. The profit margin related to each product plays a key role in this regard and it was shown that a price increase of 35% to 60% will make the flexible configurations as profitable as the least flexible one. On the contrary, for the Biochemical option, the more flexible the system is, the more profitable it will be.

In both options, the effect of flexibility on lowering the sensitivity of the system's profitability on feedstock, energy, and product prices is considerable. In Thermochemical option, the ability of shifting from a less profitable product to a more profitable one enables reducing the sensitivity on product price. The same rule is valid for Biochemical option. Moreover, flexibility increases the cash flow of the Biochemical option and thus makes it less vulnerable to price changes.

The Thermochemical strategies result in lower IRR compared to Biochemical strategies, but they have higher robustness against market volatility. Biochemical option needs more capital investment, but via the phased approach, the capital spending is divided into three phases. 45% of capital spending is done in the first phase, 47% in the second phase and the rest in the third phase. The division of capital spending for Thermochemical option is different. 70% of capital is spent in the first phase, while second and third phases each takes 15% of capital. Therefore, the capital spending is better divided over the implementation period in Biochemical option and this can be a competitive advantage for this option.

CHAPTER 4 GENERAL DISCUSSION

Over the past few years, forestry industry in North America have been facing significant challenges related to a declining and volatile market demand, growing competition from global low-cost producers, increasing competition for feedstock and market share, considerably high energy cost, strict regulations and high environmental expectations from the public. We must add to these the capital intensiveness of the industry and its aging mills and equipment. Lack of R&D activities in forestry companies have resulted in a low level of innovation in terms of developing new products and new ways of doing business. Hence, forestry companies are driven to seek alternative business models to be competitive over the longer term. On the other hand, having the required utility systems in place and the engineering know-how, existing feedstock supply chain networks and product delivery systems, as well as the potential for mass and/or energy integration between existing processes and new processes imply competitive advantages for the forestry companies to improve their economic performance. In other words, the aforementioned advantages provide the opportunity of implementing new processes along with the existing processes.

One alternative for forestry companies is to enter the bio-energy and biorefinery sectors that have been emerging in recent years. More specifically, the forest biorefinery (FBR), i.e. a category of biorefineries which primarily aims to process forest biomass as raw material, typically in retrofit to existing pulp and paper (P&P) mills, is viewed as a strong option. Therefore, the starting point for a forestry company willing to enhance its economic performance is to take a strategic view of transforming its core business to FBR by producing new products and by changing the way of doing business, given its competitive advantages.

For the FBR to be successful, in the short term, companies should focus on improving their margins by implementing a *margins-based SC operating policy* and better exploiting the process capability for *flexible production*, to mitigate the risks of market volatility. Supply chain (SC) analysis carries out product planning over different time horizons and identifies tradeoffs between product orders and anticipated supply and demand. It calculates the profit across the entire SC and accounts for cost contributors that are typically ignored in economic analyses, e.g. inventory cost and changeover cost. It can also be used to take into consideration market volatility, and determine how the flexibility of the manufacturing system can be exploited to mitigate market risks in order to maximize profit. Over the long term, companies should base their strategic decisions on a bottom-up approach, i.e. to design the SC based on the effect of the design on operational activities. SC analysis can be used to target the desired level of flexibility of a manufacturing system needed to mitigate the risk of market volatility. Moreover, these capabilities provide better insight into the costs and profit incurred by an implemented strategy. Thus, an SC analysis can be used, not only for making mid- and short-term decisions related to the management of the SC, but also for making long-term design decisions. By bringing up the operational issues of a manufacturing system to the design level, SC analysis can be employed at the strategic level for:

- Targeting the level of flexibility of a manufacturing system
- Designing the SC network of a company
- Comparing several strategies, that can be pursued by a company, by evaluating their performance for different market conditions

A design methodology including an SC-based analysis that can reflect the effect of operational activities at the design stage is proposed. The goal of this research is therefore to illustrate a design methodology for targeting the level of flexibility, designing the SC network, and evaluating different FBR strategies for transforming a forestry company. The methodology uses a generic operational SC optimization model developed for biorefineries that can evaluate the performance of strategies at the operational level. A set of performance metrics representing SC profitability, robustness and flexibility is used to evaluate the performance of biorefinery strategies for several market scenarios and to identify the promising ones. The methodology is demonstrated using a case study that involves two product/process options, including thermochemical and biochemical processes, with a few number of implementation strategies implemented over several years.

4.1 Margins-based policy vs. Manufacturing-centric approach

In order to mitigate the risk of market volatility, biorefinery operations must be run in a way that profit is maximized across the whole SC. For this purpose, the potential for flexibility throughout the SC must be exploited. Margins-based operating policy can very well attain this goal by identifying, on one side, the costs associated with all SC activities, and on the other side, the most profitable orders. Exploiting the flexibility of processes is of crucial importance in this regard. Flexibility in product and volume helps the margins-based policy to produce the most profitable products in the right volume at each time period.

The cost associated with applying such operating policy is often higher than the traditional manufacturing-centric approach, which tries to minimize the costs. But margins-based policy compensates the cost increase by improving revenue, and thus the net profit is always higher compared to the traditional approach. In some cases that the market is weak, the cost incurred by the margins-based approach might be lower than the cost associated with the manufacturing-centric approach. Therefore, margins-based policy tries to maximize profit either by maximizing revenue, or by minimizing costs. This approach adds significantly to the profit of the systems which produce added-value products. It also improves the profit of commodity production systems, though this profit improvement is not very considerable. However, as there is no extra cost associated with this approach at the design level, it is still worth applying the margins-based approach for commodities.

Elasticity of product prices is another issue that must be considered. Generally, commodities do not have high price elasticity. Therefore, changing the production volume doesn't affect their price. But, products with high value and high price elasticity would lose their value, if their production during a weak market period is continued with the same rate as it is in normal conditions. Therefore, applying margins-based policy can be more important when price elasticity is considered. However, if the price elasticity of a high value product is low, there will be no difference between the results of margins-based and manufacturing-centric policies.

4.2 Developing metrics for evaluating the performance of the SC

There are several issues regarding the performance of SCs that must be quantified, so that different alternatives can be compared with each other, or a specific SC can be designed based on the performance quantification. SC metrics are developed and used for this purpose. In this work, four SC metrics are introduced or used for evaluating the performance of SC. SC profitability in the form of internal rate of return (IRR) as a metric that is rarely used in SC analysis, is applied to show the long-term performance of an SC alternative. On one hand, in SC studies, SC profit is generally used as a measure, which is not enough, as it does not consider the capital cost required for designing the SC. Net present value (NPV) is used often when profitability is considered in SC analyses. On the other hand, in economic analyses, SC considerations are typically ignored. More specifically, some major cost contributors such as inventory cost are not taken into account. To have a better cost representation, IRR is considered in this work. It must be mentioned that IRR is not calculated directly by the SC optimization. SC profit is calculated by the SC optimization and, using the capital cost, the IRR is calculated.

Another metric that is introduced is the metric of robustness (MR). By calculating the deviation of downside profits from the base-case profit, this metric represents the robustness of the system against market volatility. Unlike typical robustness metrics that give average deviations, e.g. standard deviation, the proposed metric consider the number of downside scenarios, so that it can provide a more interpretable value. Metric of flexibility (MF) is another metric that is defined to address the volume flexibility of processes explicitly and their product flexibility implicitly. It calculates the deviation of process operating rate from its nominal value for all products that are produced. A conditional value-at-risk (CVAR)-type parameter is also introduced to show the level of risk associated with sales strategies in terms of making contract versus selling products on spot.

These metrics are used to evaluate the design of SCs by providing a trade-off between SC profitability and its flexibility as well as robustness. The results show that robustness always improves by increasing flexibility, which is due to the increasing capability of process in shifting from a non-profitable operating mode to a profitable operating mode. Moreover, higher flexibility improves the profit. However, the effect of flexibility on profitability is not obvious, because, besides profit, there is another component in profitability, which is capital cost. A flexible process is always more expensive than a non-flexible process. In other words, a flexible process needs more capital cost. Therefore, for a flexible process to be profitable compared to a non-flexible process, the profit improvement incurred by the flexibility must compensate the extra capital cost paid for more flexibility. In this regard, the profit margin associated with each product is very important.

4.3 Targeting the design of process flexibility

As being flexible is a critical point for margins-based policy, targeting the level of process flexibility is critical. Margins-based policy maximizes the profit by exploiting flexibility and considering all SC activities. Therefore, in targeting the design of process flexibility, it is not only the process-related costs that must be addressed, but also all SC costs as well as market requirements and market volatility must be taken into account.

The linkage between SC optimization and process flexibility considerations has been made mainly for tactical/operational purposes, i.e. how to exploit the flexibility of processes in order to maximize the SC profit. The classic approach for targeting the design of flexibility was to do a trade-off between level of flexibility and its associated cost. This cost implied the costs related to processes modifications required for increasing flexibility. Targeting the design of processes through a SC analysis has not been addressed before.

A step-wise methodology is pursued for targeting the level of flexibility. The methodology is fed by the separate methodologies on identifying the most promising product/process portfolios. Followed by chemical engineering heuristics, a few number of process alternatives, representing different potentials of flexibility, are defined. In parallel with that, SC network alternatives are defined based on the specifications of new products, the existing SC assets, process alternatives, and company's strategies, advantages and disadvantages. Then, process alternatives and SC network alternatives are combined and their required capital cost is calculated. Next, different levels of flexibility, i.e. operating window, are defined for the processes of each combined alternative and finally, the SC model is run for each operating window of each combined alternative in case of several market scenarios representing market volatility. The results are quantified using the developed metrics. The best operating window can be identified.

The results show that flexibility is critical for a robust design and it improves the robustness of a system in response to market volatility. With the proposed approach, the cost of flexibility can be calculated and it can be illustrated that at what level of flexibility, having flexibility matters, i.e. the extra capital cost paid for having a higher level of flexibility is compensated by enhancing system's capability facing with market volatility. Moreover, using SC analysis, the optimum production sequence of flexible processes, which is not obvious, is identified and a better representation of costs will be provided for decision making by taking cost contributors such as inventory cost and changeover cost into consideration.

4.4 Designing the SC network using a scenario-based approach

Designing the SC network consistent with process flexibility is very important. There is a direct relationship between level of flexibility, and the configuration and specifications of the SC network.

A specific level of flexibility affects the strategies in sales, partnership and transportation. It is shown by the results that when the flexibility of the processes is increased, the production capacity of products changes. In this case, some new opportunities might be found for the company in the market. That will change the strategies of the company, because the new opportunity may imply a specific partnership, sales strategy, new warehouses or new transportation system or strategy. Moreover, a specific level of flexibility requires a specific inventory limit and transportation capacity. These are SC network design issues that are linked to and affected by the process considerations. Hence, there must be integration between targeting the level of process flexibility and designing the SC network.

In the real world, forestry companies face limited options in terms of future strategies, product/process options, access to biomass, product market, etc. These all limit the choices of a company for its future. Therefore, instead of using large-scale SC mathematical formulations which consider thousands of options, a practical scenario-based approach can be used to identify the possible options and to evaluate their performance in the long run.

4.5 Phased implementation approach

Implementing biorefinery through several phases can reduce the risks associated with immaturity of product market and technologies, and also lack of capital. Company's policies and limitations must be considered in the definition of phases. Again, SC analysis reflects the market volatility into the economic analysis related to phased implementation strategies and gives a better cost representation compared to usual economic measures.

CHAPTER 5 CONCLUSIONS AND RECOMMENDATIONS

5.1 Contributions to the body of knowledge

A systematic design methodology for designing the SC of biorefineries

- Separating the SC design into targeting the level of process flexibility and designing the SC network
- Potential for being integrated with product portfolio definition and techno-economic methodologies and providing information/criteria along with other analysis tools such LCA for an MCDM framework
- Bringing the SC operational considerations up to the strategic decision-making level in order to analyze the effect of design decisions on the operational issues
- This methodology claims to be effective for practical and industrial projects and case studies. In fact, a company-based view is taken in this methodology to provide a systematic design framework which is not very complicated for industry, and at the same time, can help solve real-world problems using the latest advances in SC optimization and systems engineering.

Concretizing the concept of margins-based operating policy in the FBR

- Showing the value of margins-based operating policy in improving the profitability of biorefineries compared to traditional manufacturing-centric approach for both commodity chemicals and value-added products in different market conditions

Introducing metrics for evaluating the performance of SC

- SC profitability metric considers all cost contributors in profitability analysis and gives a better cost representation of the system compared to usual economic metrics which only focus on process-related costs.
- Metric of robustness provides a simple representation of robustness by measuring the deviation of downside profits from the base-case profit.
- Metric of flexibility quantifies volume flexibility and implicitly implies product flexibility. It shows the deviation of production volume from the nominal production rate for all products.

- CVAR-type parameter can be used for analysing risks associated with sales strategies, i.e. how the production capacity must be dedicated to contractual orders and spot orders and what percentage of contractual orders must be accepted and fulfilled.
- All these metrics together can be used for analyzing the performance of an SC and for determining which level of flexibility in processes and which SC network configuration will have a better performance at the operational level.

Targeting the level of process flexibility using an SC-based analysis

- Instead of taking into account only process consideration and process-related costs in designing/targeting the level of flexibility, all SC constraints including procurement, inventory and transportation constraints, and SC costs are considered.
- Market volatility is also reflected to this problem by analyzing the value of robustness metric and its change relative to the level of flexibility. The ultimate goal is to target the level of flexibility so that the deviation of downside profits resulted from different market scenarios from the base-case profit is minimum. In other words, the aim is to find a level of flexibility that minimizes the risk of market volatility.
- SC profitability and metric of robustness in conjunction with metric of flexibility targets the desired level of flexibility.

Applying a scenario-based approach for designing the FBR SC

- To account for the restrictions and policies of the company, a scenario-based approach is proposed for designing the SC network.
- With this approach, engineering heuristics can be properly integrated with SC design. Process alternatives, representing different potentials for flexibility, are defined based on chemical engineering practices.
- SC network alternatives are defined, on one hand, according to defined process alternatives, and on the other hand, based on the constraints of the company and its potentials.

To sum up, the methodology developed in this thesis exploits margins-based policy, after proving its value, to target the design of biorefinery process flexibility and to design the biorefinery SC network. Ultimately, the methodology is intended to be used to identify the implementation strategy of biorefinery, considering the effects of such strategic decisions at the operational level activities. To the best of our knowledge, no previous research to date has focused on such issues in the context of biorefinery.

5.2 Future works

5.2.1 Overall methodology

This methodology is linked to product portfolio definition and techno-economic studies and uses the output of such methodologies. It provides metrics and criteria that can be used in MCDM frameworks. A potential future work is to focus on the way that this methodology can be integrated with LCA, both environmental LCA and social LCA, in order to address the sustainability issues of the biorefinery.

5.2.2 Operability/controllability

The proposed methodology does not aim at designing the flexibility of processes. It addresses a step behind the design stage, which is targeting the design of flexibility. For designing the targeted level of flexibility, operability and controllability issues must be considered. These considerations can be categorized into two classes;

- Those which are related to the design of the process, i.e. investigating whether the targeted operating window is feasible from a controllability perspective or not. In other words, it must be verified if the process is controllable within the targeted operating window.
- Those which are related to operational issues. Changeover cost and time were issues considered in the SC formulation presented in this work. Operability and controllability studies analyze the transition time from one steady-state operating point to another steady-state operating point. Thus, they can provide better information about the time losses during a changeover, and thus, the cost incurred by that.

Therefore, operability and controllability studies can be carried out for the next step of flexibility design.

5.2.3 Incorporating the concept of uncertainty

The uncertainty was considered in this work through scenario generation. Probability was not taken into account, except in the Monte Carlo simulation carried out for analyzing the profitability of implementation strategies. Therefore, a deterministic approach towards uncertainty was taken in this methodology.

Addressing the issue of uncertainty with a stochastic approach can be brought into this problem via upgrading the mathematical formulation to a two-stage stochastic formulation. Design decisions can be determined by such formulation, instead of being defined using heuristics. A two-stage stochastic formulation is quite relevant to this type of problem. There are three major issues that can be addressed by a two-stage formulation: targeting the level of flexibility, designing the SC network, and identifying the most promising capacity expansion strategy. These decisions are made using scenarios and heuristics in the methodology introduced in this thesis.

The CVAR parameter also implies opportunities for future works. This parameter was not involved in the developed methodology. Along with metric of robustness, it can be integrated with metric of flexibility to analyze the risk and robustness of different levels of flexibility.

5.2.4 Upgrading SC model from operational planning level to strategic design level

The SC model can be upgraded from an operational planning model to a simultaneous planning-design model. A few number of design variables can be added to the model to upgrade it. The efficiency of the model in terms of running time must be investigated. The current model is run for every week. For a design problem, especially to include capacity expansion planning, a time horizon of several years must be taken into account. Thus, the model must be run for every week over several years. That would dramatically enhance the size of the problem.

The following binary variables, parameters, equation and constraints can be added to the SC formulation so that it can be used for, not only making operational decisions, but also design decisions.

Parameter

c_{lpt}^{cap} Investment cost of process *p* in mill *l* implemented from time period *t*

CP_l Construction period of process *p*

Decision variable

δ_{lpt}^{proc} Implementation of process *p* in mill *l* in time period *t*

γ_{lpt}^{proc} Installation of process *p* in mill *l* in time period *t*

Objective function

$$\max CCF = \begin{pmatrix} Revenues - ElectricityCost - SalesCost \\ -VariableOpCost - FixedOpCost - ChangeoverCost - ShutdownCost \\ -TransportationCost - StorageCost - ProcurementCost \\ -InvestmentCost \end{pmatrix}$$

Investment costs are equal to the sum of capital investment of each process implemented in from a time period.

$$InvestmentCost = \sum_{t\in T>1} \sum_{\{l,p\}\in P^L} (\delta_{lpt+1}^{proc} - \delta_{lpt}^{proc}) c_{lpt}^{cap}$$

Constraints

Equation $21'$ mandates that a recipe is used on a process that is installed.

$$\alpha_{lprt}^{rec} \leq \delta_{lpt}^{proc} \quad \forall \ \{l,p,r\} \in R^P, t \in T \tag{21'}$$

Equation $21''$ means that a process can operate in a time period only when it is installed. Production must start after the construction period (CP_l) ends.

$$\delta_{lp(t+CP_l)}^{proc} \leq \sum_1^t \gamma_{lpt}^{proc} \quad \forall \ \{l,p\} \in P^L, t \in T - CP_l \tag{21''}$$

Equation $21'''$ensures that no process can operate over a period equal to CP_l starting from t=1.

$$\sum_1^{t=CP_l-1} \delta_{lpt}^{proc} = 0 \quad \forall \ \{l,p\} \in P^L \tag{21'''}$$

Equation ($21''''$) ensures that when a process is installed, it operates over the remaining time periods.

$$\delta_{lpt-1}^{proc} \leq \delta_{lpt}^{proc} \quad \forall \ \{l,p\} \in P^L, t \in T > 1 \tag{21''''}$$

With the proposed items, the SC formulation will change to a simultaneous design-operational planning SC formulation and can be used for capacity expansion planning problems, in which the installation time of each process and its capacity is determined.

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APPENDICES

APPENDIX A – Article: Integrating product portfolio design and supply chain design for forest biorefinery.

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APPENDIX J – Conference Paper: Metrics for evaluating the forest biorefinery supply chain performance.

APPENDIX A – Article: Integrating product portfolio design and supply chain design for forest biorefinery

Integrating product portfolio design and supply chain design for the forest biorefinery

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Abstract

Supply chain (SC) design involves making strategic long-term decisions for a company, e.g. number, location and capacity of facilities, production rates, flow of material between SC nodes, as well as choosing suppliers and markets. The forest biorefinery is emerging as a promising opportunity for improving the business model of forest product companies; however it introduces significant challenges in terms of mitigating technology, economic and financial risks – each of which must be systematically addressed in the SC design. In this regard, product portfolio definition and technology selection are two important decisions that have rarely been considered in a systematic SC evaluation. This paper presents a methodology, in which product/process portfolio design and SC design are linked in order to build a design decision making framework. According to this methodology, design of "manufacturing flexibility" links product/process portfolio design to SC design, through a margins-based SC operating policy. Techno-economic studies along with scenario generation for price and demand changes representing market volatility are employed in the methodology.

Keywords

Forest Biorefinery, Supply Chain Design, Product Design

1. Introduction

Pulp and Paper (P&P) companies in Canada are facing a stalemate situation (Stuart, 2006). Their business has been endangered by global low-cost competitors; they are encountering declining markets and over capacity. In order to remain low-cost producers, they have cut operating and labor costs as well as R&D activities and spent minimum capital to modernize their mills which ultimately have resulted in a lack of knowledge about product quality requirements and supply chain (SC) practices. What seems to be critical for forestry companies in this situation is, not only, diversifying the revenues by producing more value-added products, but also changing the

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current manufacturing culture existing in this arena. These strategic changes imply Enterprise Transformation (ET) (Chambost et al., 2008). ET implies evolving corporate-wide initiatives designed to impact the strategies, structures and human system of the corporation – as well as to create more sustainable and profitable organizations. ET must be performed in two distinct ways referenced as “inside-out” and “outside-in”. Inside-out transformation is when the current mission/vision of the company is kept unchanged and the company is made-over in terms of its processes and manufacturing culture. Outside-in transformation involves changes in current mission/vision and the core business of the company by producing new products and providing new services.

One possible strategy that forestry companies are considering is to transform their pulp and paper mills into integrated forest biorefineries (FBR). The American National Renewable Energy Laboratory (NREL) published the definition: “A biorefinery is a facility that integrates biomass conversion processes and equipment to produce fuels, power, and chemicals from biomass” (NREL). Various FBR process technologies are under development based on chemical routes (e.g. lignin precipitation), thermochemical routes (e.g. biomass gasification) and biochemical routes (e.g. hemicellulose fermentation) (Wising & Stuart, 2006). These technologies can potentially be integrated into existing P&P mill facilities resulting in significantly reduced capital costs for implementing the FBR. Forestry companies can potentially transform their business model by implementing the FBR, and produce bioproducts besides P&P products, which implies outside-in transformation. On the other hand, FBR implementation will change the company's core business; therefore they need new management practices and manufacturing culture, which implies also inside-out transformation.

FBR implementation can be performed based on a strategic phased approach which can be considered by P&P companies, Figure 1(Chambost et al., 2008).

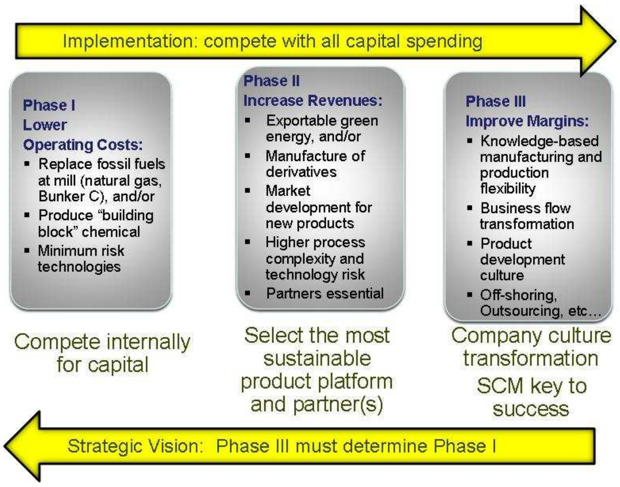

Figure 1. Strategic implementation of the biorefinery by a P&P company

In phase I, companies must lower their operating costs by producing substitute fuel products for fossil fuels such as bunker C or natural gas. Such projects must compete internally for capital due to lack of capital spending budget in P&P companies. In phase II, companies increase their revenue by producing and selling one or more value-added products that enlarge their existing product portfolio. This phase includes considering the production of new value-added products as part of the core business, which in turn implies outside-in transformation. The main challenge at this phase is to select the most sustainable product/process portfolio. In phase III, companies focus on improving margins through knowledge-based manufacturing. Knowledge-based manufacturing involves using detailed knowledge of process capability for flexible production, and advanced SC optimization techniques for product planning over different time horizons and identifies the trade-offs between product orders, anticipated supply and demand and manufacturing flexibility. As these activities seek improved bottom-line results via transforming the enterprise in terms of work and process steps, phase III implies an inside-out transformation (Chambost et al., 2008).

Producing several products implies the opportunity of taking advantage of manufacturing flexibility via the identification of new product portfolios at a given mill. (Chambost et al., 2008). In a volatile market, according to the feedstock and product price as well as supply and demand constraints, the manufacturing flexibility can be exploited via a margins-based SC operating policy to produce different products in different amounts in order to optimize and secure the company's margin. Hence, the challenge in phase III is to develop a SC-based analysis which can be used to, firstly, design the SC network so that it can serve the margins-based SC operating policy at tactical-operational levels and, secondly, improve the company's margins via exploiting the manufacturing flexibility.

Given the phased approach presented above, there are two critical aspects for the FBR implementation, i.e. product/process portfolio definition and SC network design. What links these two aspects is the design of "manufacturing flexibility". At the first step, considering volatility in the market, product/process portfolio must be defined for enabling the company to be flexible enough to stabilize the margins via the margins-based operating policy. Afterwards, the range in which the production rates can vary must be determined for each process. This range would be a design target for each process and the process must be designed so that the system can handle the targeted flexibility. Finally the SC network must be designed so that the market requirements can be met through the designed SC network and within the designed range of production rate.

The goal of this paper is to propose a hierarchical methodology for a SC-based analysis which can integrate these three aspects, i.e. product/process portfolio design, design of manufacturing flexibility, and SC network design. The proposed methodology will be able to evaluate product/process portfolio options and the required manufacturing flexibility, and to reflect them in the SC network design. The decision as to what biorefinery strategy to take depends on many factors most of which cannot be reflected in a practical manner in an optimization problem. Examples of such factors are mutual interests of potential partners in a joint venture company, or the competitive disadvantages of forestry companies such as a lack of capital. Thus, this methodology seeks a set of feasible and practical biorefinery options, not the best one, which can be strategically pursued by a company. It can be employed to identify possible options that should be addressed in further strategic decision making steps.

This paper is organized as follows. First, the previous studies in integrating product, process and SC design are reviewed. Then, the concepts used in the methodology, i.e. product portfolio, margins-based SC operating policy, manufacturing flexibility, SC management and SC model, are defined. Afterwards, the methodology is presented. Each step of the methodology is described and the way in which SC modeling is used at each step is explained. Finally, an illustrative example is introduced and the results presented to highlight the importance of implementing the proposed methodology.

2. Product, process and SC design

Integration of product, process and SC design has not gained attention in the chemical engineering context. The majority of articles in the body of literature relate to discrete manufacturing and assembly process environments, e.g. car and electronics manufacturers. This integration has been studied in computer and notebook manufacturing (Huang et al., 2005), aviation electronics (Blackhurst et al., 2005) and car manufacturing Lamothe et al. (2006).

In the context of biorefinery, Sammons et al. (2008) proposed a general systematic framework for optimizing product portfolio and process configuration in integrated biorefineries. The framework first determines the variable costs as well as fixed costs using data in terms of yield, conversion and energy usage for each process model. Next, process integration tools, e.g. pinch analysis, are employed to optimize the models. Finally, the optimized model will generate data for economic and environmental performance metrics. An optimization formulation enables the framework to decide whether a certain product should be sold or processed further, or which processing route to pursue if multiple production pathways exist for a special product. However, it seems that this methodology does not involve market investigations before selecting the products and no SC metric is considered in the framework. These points might question the practicality of the proposed methodology.

3. Concepts and definitions

3.1. Product portfolio

The goal of the forest biorefinery is to increase revenues through the production of non-traditional chemicals – biofuels and added-value biochemicals implying the diversification of the existing product portfolio (traditional pulp and paper products). The new revenue streams may be from the development of a biorefinery product family based on key building blocks and their related derivatives with existing P&P production (Chambost et al., 2008). Defined by Meyer (1993) as a set of products that share a common platform, but have specific features and functionalities required by different sets of customers, the forest biorefinery product family implies the strategic definitions of product/process combinations, product delivery to the market and competitive position of product on the market. The flexibility of the product family is essential in order to successfully face market volatility and mitigate market risks. The modified product portfolio, comprising the new product family and the existing pulp and paper production, might be implemented gradually one project at a time, at several mills, and support the creation of value over the long term. The development of the new product portfolio might lead to several benefits such as adjustment of supply to the market for mitigating market risk using process flexibility, stabilized margins and secure return on the long term.

3.2. Margins-based SC operating policy

The operating policy in the P&P industry is said to be “manufacturing-centric”. In this industrial sector, management focus is on capacity and industry participants have been managing the efficient and effective use of machine capacity (Lail, 2003). As a result, process efficiency is viewed as the key measure for profitability and thus it is believed that minimizing production cost will result in the highest profitability (Dansereau et al., 2009). Also, production planning assumes known orders and fixed sequence of product grades. Treating the manufacturing process as the focal point, inventory and change-over costs are typically ignored or considered separately (Lail, 2003) and SC costs are often neglected resulting in less profitability (Dansereau et al., 2009).

In order to implement the FBR, the operating policy must change from the manufacturing-centric approach to a margins-based one. This operating policy tries to maximize the margins over to entire SC and to produce/select products/orders that ensure the best returns (Dansereau et al., 2009).

3.3. Manufacturing flexibility

Sethi and Sethi (1990) did a comprehensive survey on the concept, different definitions and types of manufacturing flexibility. They defined flexibility of a system as its adaptability to a wide range of possible environments that it may encounter. In the chemical engineering context, Grossmann et al. (1983) defined flexibility as the ability of a manufacturing system to satisfy specifications and constraints despite variations that may happen in parameter values during operation. What is common among all types of flexibility is that flexibility is employed to mitigate the risks associated with different types of uncertainty. These uncertainties are the results of variations in the temperature, pressure, or flowrate of a stream, state of equipments, or fluctuations of price and demand of products. Based on the type of uncertainty, a specific type of flexibility can be defined. Browne et al. (1984) classified the manufacturing flexibility in the discrete manufacturing environment into eight different categories, i.e. machine, process, product, routing, volume, expansion, operation and production.

Table 1. Types of flexibility and their definition

Flexibility	Definition
Recipe	The ability of having a set of adaptable recipes that can control the process output
Process	The ability of process to operate on a range of conditions and to handle the disturbances
Product	The ability to changeover to produce a new (set of) product(s) economically
Volume	The ability to operate a system profitably at different production volumes

In the chemical engineering context four major types of manufacturing flexibility can be considered, i.e. recipe, process, product and volume. These definitions are illustrated in Table 1.

3.3.1. Flexibility of recipes

Flexible recipe concept was originally introduced as a set of adaptable recipe items that can control the process output, and can be modified to confront any deviation from the nominal conditions. Recipes prescribe how products are to be produced. According to the production scenario, recipes can be changed or modified. Verwater- Lukszo developed this basic idea and introduced the concept of flexible recipe as a way of systematically adjusting the control recipes during the execution of the production tasks with the aim of enabling the process to perform under different operating conditions (Verwater-Lukszo, 1998). One of the first attempts was done by Romero et al. who extended the flexible recipe approach to a plant-wide scheduling problem (Javier Romero et al., 2003). Another work was done by Ferrer-Nadal et al. who aimed to optimize the production scheduling of a batch plant where flexible recipes were employed. Laflamme-Mayer et al. (2008) developed a SC planning model that exploits the capability of a market pulp mill in using different recipes in a flexible manner in order to provide adequate support for cost effective fiber supply.

3.3.2. Process flexibility

In the chemical engineering context, process flexibility has gained more attention. From a general point of view, process flexibility is a property of “process operability”. Wolff et al. (1994) broke down the operability into a set of properties such as stability of the plant, optimality, selection of measurements and manipulated variables, flexibility and controllability.

Bahri, Bandoni & Romagnoli (1996) named flexibility and controllability as two major concepts in operability assessment. Flexibility is concerned with the problem of ensuring feasible operation of a plant for a whole range of conditions in both steady-state and dynamic environments, while controllability signifies the ability of a plant to move efficiently from one operating point to another as well as dealing efficiently with disturbances.

Flexibility, as a property of operability, has been studied broadly. Grossmann et al. (1983) gave an overview of the chemical process design problems in which the existence of regions of feasible steady-state operation must be ensured in the face of parameter variations. Two major areas have been considered by them: optimal design with a fixed degree of flexibility, and design with optimal degree of flexibility. Optimal design with a fixed degree of flexibility deals with the problems in which the required flexibility has already been specified, either by a discrete set of required operating conditions or by requiring feasibility of operation when a set of uncertain parameters can vary between fixed bounds (Grossman, 1983). On the other hand, design with optimal degree of flexibility is faced with problems which need a trade-off between the cost of the plant and its flexibility. Therefore the objective would be to minimize capital and operating costs on one side and to maximize flexibility on the other side (Grossman, 1983). Problems in this category have evolved from flexibility index problems (Swaney & Grossmann, 1985), to stochastic flexibility index problems (Pistikopoulos & Grossmann, 1988) and expected stochastic flexibility index problems (Straub & Grossmann, 1993).

3.3.3. Product/Volume flexibility

Some manufacturing systems use the combination of different types of flexibility. This approach is widely used in the refineries and the petrochemical industry. Petrochemical complexes are able to produce several products via processes which can operate in a range of production rates. Neiro & Pinto (2004) and Schulz et al. (2005) described SC planning of petrochemical complexes which employ this strategy. Mendez et al. (2006) explained the scheduling of oil-refinery operations where continuous processes produce some components with constant flowrates and then a blending process is used to transfer those components into different derivatives in variable amounts.

Finally, it is worth noting that manufacturing flexibility contributes to the flexibility of the whole SC. The flexibility of a SC involves the flexibility of all its nodes, i.e. suppliers, manufacturers, warehousing and transportation centers.

3.3.4. Manufacturing flexibility in the FBR

The concept of flexibility used in this work implies the ability of producing several bioproducts with different production rates in different time periods based on the product price and demand. From an economic perspective, this type of manufacturing flexibility implies a justifiable increase in capital cost that is adequately compensated in the ability of the process to manufacture with flexibility, such that expected volatility in market conditions can be mitigated. The proposed definition seems to be the aggregation of product flexibility and volume flexibility. As process flexibility is inherent in the design of each chemical process, this definition has already included process flexibility. Thus the definition of manufacturing flexibility in this work can be interpreted as the aggregation of process, product and volume flexibility. In fact, many types of flexibility are the aggregation of others (Sethi & Sethi, 1990). As discussed by Jaikumar (1984), flexibility in manufacturing is always constrained within a domain which should be defined in terms of portfolio of products, process, and procedures and should be well understood by product designers and manufacturing engineers.

In the FBR, there is a promising opportunity for implementing the defined manufacturing flexibility. As mentioned in the introduction, the FBR processes can be retrofitted to P&P mills which are in place with a known level of flexibility. The FBR and P&P mills might be integrated in terms of feedstock, chemicals and energy. Hence P&P process flexibility can be characterized and then the FBR process and its flexibility can be designed based on the flexibility of P&P side, market price and demand. This will provide the opportunity of producing both P&P products and bioproducts which will improve P&P companies' business model and might prevent current mill closures (Stuart, 2006).

3.4. Supply chain management (SCM)

Supply Chain Management (SCM), as phrased by Guillen et al. (2006), aims to integrate manufacturing facilities with their suppliers and customers so that they can be managed as a single entity and to coordinate all input/output flows, i.e. flow of materials and information, so that products are produced and distributed in the right quantities, to the right locations, and at the right time. The main objective of the SCM is to achieve acceptable financial returns along with the desired consumer satisfaction levels.

The SCM problem may be considered at different levels depending on the level of the SC on which it is applied, i.e. strategic, tactical and operational. The strategic level addresses long-term decisions on the SC design, and involves determining the optimal configuration of the entire SC network, i.e. determining the number, location and capacity of all SC nodes and choosing suppliers and target markets (chopra & Meindl, 2007). The tactical level includes mid-term management decisions, which must be typically made on a monthly basis. Examples of such decisions are overall purchasing and production decisions, inventory policies, and transport strategies (Guillen et al., 2006). The operational level comprises day-to-day decisions such as production scheduling, lead-time quotations and routing (Guillen et al., 2006).

3.5. Supply chain model

A SC model aims to calculate the optimum profitability of the whole SC. It aims to maximize the profitability across the entire SC by finding the optimal alignment of manufacturing capacity and market demand. It is formulated into an optimization problem whose objective function is the sum of revenues subtracted by the SC costs including feedstock, inventory, production, transition and shutdown costs. There are two types of decision variables in the mathematical formulation of the SC model. The first type is continuous variables which comprise flow of material between SC nodes, amount of each product that must be produced, and the inventory levels. The second type is binary variables which imply “yes/no” type of decisions, e.g. if a product must be produced or a production line must operate. Each node of the SC, i.e. suppliers, inventories, manufacturing centers, has some constraints which must be formulated mathematically. The SC model applied in this work is used at two different levels, i.e. tactical planning and operational scheduling.

4. Methodology

The hierarchical methodology proposed in this paper comprises three major steps each of which point out one of the three key aspects mentioned previously, i.e. product/process portfolio design, design of manufacturing flexibility, and SC network design (Figure 2). The first step deals with product/process portfolio design through product portfolio definition and Large Block Analysis (LBA). The second step implies designing the manufacturing flexibility. The third step addresses the SC network design which involves redesigning the SC network configuration.

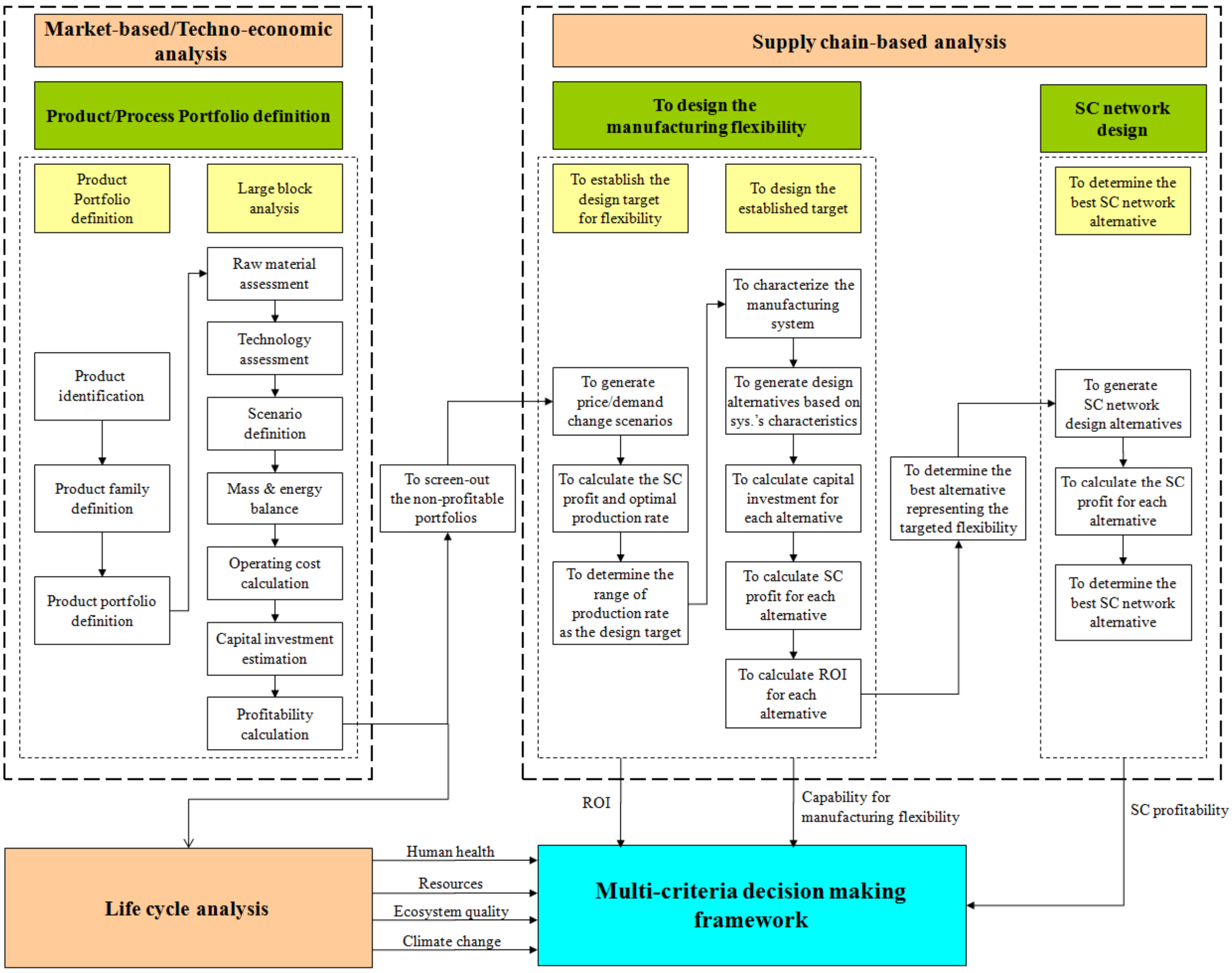

Figure 2. Product/Process portfolio definition

The specific objectives of each step will be as follows:

- First step: Defining product/process portfolios
  - Products to be produced
  - Processes to be employed
- Second step: Targeting and designing the required manufacturing flexibility
  - Specifying the range of production rate for each process
  - Designing the production lines which represent the targeted flexibility
- Third step: SC strategic network design

- Determining the mill locations, warehouse and distribution centers expansions, new warehouse and distribution centers locations and allocation of distribution centers to markets

4.1. First Step: Product/Process Portfolio Design

At this step, the challenge is to identify the most promising product/process combination from a large range of product/process opportunities. Therefore this step can be divided into two consecutive parts; (1) product portfolio definition, (2) LBA for the defined product portfolios in order to generate product/process portfolios.

4.1.1. *Product Portfolio Definition*

A three-stage methodology has been developed for the definition of product portfolio, Figure 2 (Chambost et al., 2008). In the first stage, sets of possible products must be identified. The product identification is based on a market-driven analysis reflecting the commercial product opportunities. In this regard, products could be classified into three groups; (a) Replacement products which are identical in chemical composition to the existing products in the market, but made out of renewable feedstock, e.g. biopolyethylene. (b) Substitution products which have different chemical composition, but the same functionality, e.g. polylactic acid (PLA) instead of polyethylene terephtalate (PET). (c) Novel products like biomaterials, nanocomposites which have new functionalities and therefore no existing markets (Chambost et al., 2008). All product opportunities are investigated based on market, economic and product specific information such as product functionalities, volume, market size and growth, market saturation and basic margins. In the second stage, based on market and competitiveness criteria and a preliminary techno-economic study, possible sets of product families can be identified. For instance, ethanol, ethylene and polyethylene could form a biorefinery product family, since ethanol can be converted into ethylene and further into polyethylene. At the last stage, according to a mill or company-based analysis, product portfolios will be generated. Important elements should be taken into account while considering the definition of portfolios such as follows; (a) Manufacturing flexibility is an important criterion for product portfolio definition. It must be investigated that which set of products introduces a better potential for flexibility. (b) The defined product portfolio must be able to stabilize the margins and to secure the return on investment (ROI), thus market volatility, legislation changes and other factors must be taken into consideration. (c) The definition of product portfolio should take into account the identification of sustainable partnership models, i.e. partnering with technology providers and/or chemical companies, in order to secure the SC and lower the risks of entering an existing/new value chain. At this stage, mill's specifications must be taken into consideration in order to identify the opportunities for integration between P&P processes and bioprocesses in terms of feedstock, chemicals and energy. Finally a critical risk assessment is conducted for each product portfolio.

4.1.2. *Large Block Analysis (LBA)*

The objective of LBA is to provide comparable techno-economic data such as operating cost, capital investment cost and profitability, of different product/process portfolios and then to screen out non-profitable portfolios (Janssen, 2007). LBA has seven major stages. At the first stage, which is "raw material assessment", given the defined product portfolios, list of raw materials must be identified based on their accessibility to the mills and the maximum available volume according to their cost. The second stage is "technology assessment" in which emerging technologies for producing each product must be surveyed, taking into account the mass and energy balance, type of feedstock and technological risks of each technology. At the third stage, called "scenario definition", the combinations of raw material/process/product are generated as scenarios. From raw material to product, there are different pathways and several processing routes. For instance, for bioethanol production from biomass, there are two pathways, i.e. biochemical and thermochemical. For each of these pathways, different types of processes can be used, such as gasification for thermochemical pathway, and enzymatic or acidic hydrolysis for biochemical pathway. Finally there are many technology providers for each process. Therefore each scenario includes one type of feedstock, a specific pathway, processing route and a technology provider related to the processing route, and finally products. Thus, to define scenarios, given the outcome of the last two stages, i.e. raw material and technology assessment, the specific technology provider, and hence its corresponding process type and pathway, and the required raw material for producing each product, must be identified. At this stage, the potentials of integration of selected portfolios with the existing mill must be taken into account in terms of technological fit, integration factors and risks.

At the fourth stage, "mass and energy balance" is done for each scenario based on technology provider's and raw material specific information. The fifth stage deals with "operating cost calculation". There are two types of operating costs: variable and fixed cost. Variable costs such as costs of chemicals, fuels, etc. are calculated based on the balance sheets of the processes and price information. Fixed costs involve labor cost, maintenance, insurance and taxes, and general overhead. The sixth stage is “capital investment estimation”, in which capital investment is estimated for each scenario based on published information for stand-alone bioprocesses. Then the mill’s impact will be investigated in order to identify the potentials for integration with P&P processes in terms of chemicals or energy. In this regard, the existing mill system that can be used by the bioprocesses must be defined and afterwards, the modification cost of the mill system can be estimated. In the last stage, which is “profitability calculation”, the profitability of each scenario according to the revenue from end products and by-products will be estimated by means of ROI as profitability measures. After these stages, the non-profitable scenarios will be screened out and a finite number of scenarios will be selected as product/process portfolios. These portfolios will be analyzed further so that the best portfolio can be identified.

4.2. Second Step: Designing the Manufacturing Flexibility

This part of the methodology contains two steps which must be implemented for the remaining product/process portfolios. In the first step the range of production rate for each process is established as a design target and in the second step the established target of each process is designed. In order to perform this part of the methodology the SC model is used to find the optimum production rates.

4.2.1. *Establishing the Design target of Manufacturing Flexibility*

For each process in each portfolio, there is a nominal production rate based on the result of “technology assessment” step of LBA. At this stage, the range of production rate within which the manufacturing processes must operate is determined. In other words, it must be determined that, given the price and demand volatility in the market and with the aim of maximizing the profitability, to what extent each production rate must be able to vary. For this purpose, a finite number of price and demand scenarios, representing the price and demand volatility, are generated. Then the SC tactical model is run for each scenario. The overall problem at this stage can be stated as follows. Given:

- Number and length of time intervals in a mid-term scale
- Demand and price data for each feedstock, product, market and time interval for each scenario. Scenarios will be generated in terms of pessimistic, likely and optimistic situations.
- The configuration of the SC network
- Capacity data of the nodes of the SC

- Direct cost parameters i.e. unit production, transport, handling and inventory costs

With the aim of profit maximization, find

- Production rates of each product at each plant, for all the time intervals and scenarios
- Flows of materials between the plants, warehouses and the markets

The result will determine SC profit as well as the range of production rate for each scenario and thus the flexibility needed for maximizing the margins.

At this stage, the SC model is run with no constraint on the production rate of manufacturing processes, so that the SC model can find the optimum production rate for each process based on the product price and market demand. Figure 3 shows an example.

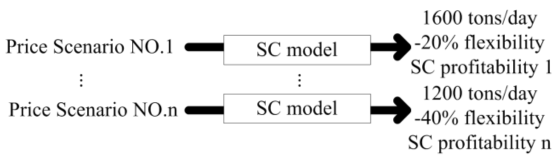

Figure 3. SC model input and output

Considering that the nominal production rate is 2000 tons/day, given a decrease in demand via scenario NO.1, the optimum production rate obtained by the SC model is 1600 tons/day, which represents -20% of flexibility based on the nominal rate (2000 tons/day), while the obtained result from SC model for the scenario NO.n, representing a stronger decrease in demand, is 1200 tons/day, which represents -40% of flexibility. This calculation must be done for each scenario in order to determine to what extent each process needs to be flexible for a given price/demand scenario. Also the SC profitability for each price scenario will be estimated and finally based on the percentage of flexibility and SC profitability the range of production rate will be determined as a design target.

4.2.2. *Designing the Established Target*

At this stage, the range of production rate will be constrained based on the result of the previous stage. For instance, given that -40% was the maximum flexibility obtained from the last stage, this percentage will be the flexibility constraint which cannot be exceeded. In other words, the SC model won't be able to go beyond this range. In order to design the targeted flexibility, the manufacturing system must be characterized based on the following aspects:

- The products can be produced in parallel lines, i.e. they are not from one family (Figure 4.a), or they can be produced in series, i.e. they are in a product family (Figure 4.b)
- The products must be produced in separate lines (Figure 4), or they can be produced in one single line, i.e. a line which is able to produce more than one product, though in different times. Sahinidis & Grossmann (1991) called this type of process a flexible production facility (Figure 5)
- The process can or cannot handle the targeted flexibility (range of production rates)

In order to clarify the way in which a manufacturing system can be characterized by these aspects, we refer to the system presented by Yun, Kim, Park & Park (2009). They presented an integrated biorefinery system which produces ethanol, lactic acid, itaconic acid and citric acid. Firstly, as these products do not belong to one product family, parallel lines are needed. Secondly all acids can be produced in one line. Thus, only two parallel lines will be needed, one for ethanol production and one for producing acids. And the third point is that the system can produce ethanol, lactic, itaconic and citric acid in the range of 6300-21000 kg/10dyas, 8720-10900 kg/10dyas, 7680-11000 kg/10dyas and 0-3840 kg/10dyas, respectively.

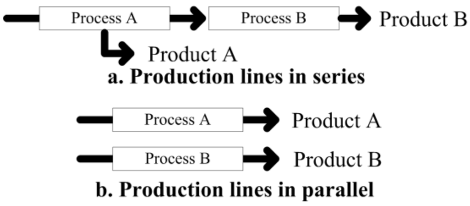

Figure 4. Separate production lines; a) in series, b) in parallel

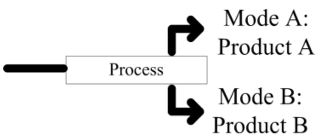

Figure 5. Flexible production line as defined by Sahinidis & Grossmann (1991)

Therefore, based on the characteristic of the manufacturing system, a limited number of design alternatives representing the targeted flexibility will be generated. Then, for each price/demand scenario, the operational SC model will be run and the SC profitability will be calculated for each design alternative. The overall problem at this stage can be formally stated as follows. Given:

- Design alternatives representing the needed flexibility
- Number and length of time intervals in a short-term scale

- Demand and price data for each feedstock, product, market and time interval for each scenario
- The configuration of the SC network
- Capacity data of the nodes of the SC
- Direct cost parameters for each SC node

Find the SC profit for each design alternative. Based on the SC profitability as well as capital investment needed for design alternatives, the ROI of each alternative can be estimated for all price/demand scenarios. Therefore, for each design alternative, SC profitability and ROI will be calculated for a set of price/demand scenarios. Based on these results, the most profitable design alternative will be identified. These steps must be performed for all remaining portfolios to identify the best alternative for each portfolio. Figure 6 shows this stage graphically.

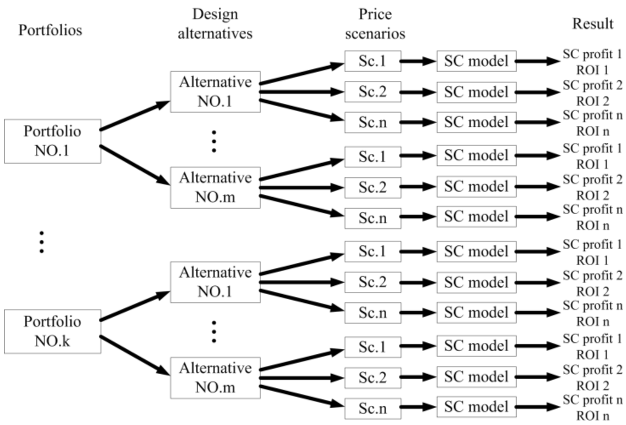

Figure 6. Identifying the most profitable design alternative

4.3. Third Step: SC Network Design

The goal of this step is to design/redesign the SC network for each product/process portfolio. For this purpose, SC network alternatives will be generated for each portfolio. Alternatives can be defined in terms of expansion of existing facilities, buying new facilities in different areas or choosing partners for product delivery. Then, given the same price/demand scenarios, or new scenarios in the case the network alternative includes new facilities in new areas, tactical SC model will be run for each SC network alternative. The overall problem at this stage can be stated as follows. Given:

- SC network alternatives
- Number and length of time intervals in a mid-term scale

- Demand and price data for each feedstock, product, market and time interval for each scenario
- Capacity data of the nodes of the SC
- Direct cost parameters for each SC node

Find the SC profit for each SC network alternative. Based on the results, the best SC network alternative can be determined for each portfolio. Figure 7 shows this step graphically.

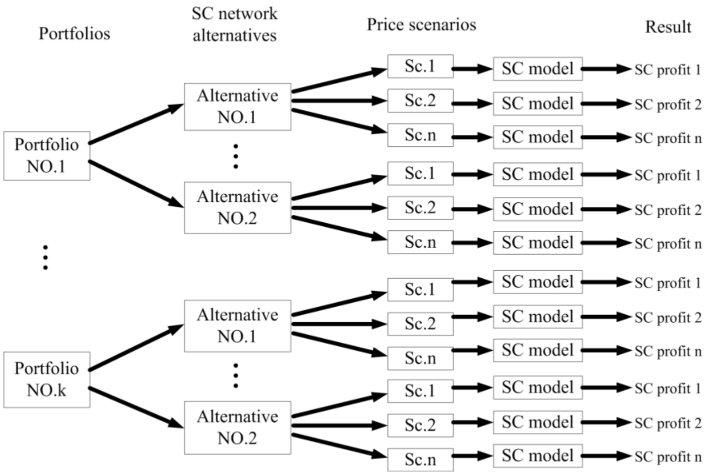

Figure 7. SC network design alternatives

4.4. Decision making framework

As it was mentioned previously, the proposed methodology must be performed for all defined product/process portfolios. After implementing this methodology, each portfolio can be characterized by means of several aspects, i.e. capability for manufacturing flexibility, SC profitability and ROI. These aspects can be used as different metrics in a multi-criteria decision making framework. It is worth mentioning that all of these metrics would be considered as SC metrics. Another metrics can be provided by Life Cycle Analysis (LCA) and added to the framework in order to address the environmental aspects of each portfolio. Based on the result obtained by the multi-criteria decision making framework the best product/process portfolio can be determined (Janssen, 2007).

5. Illustrative example

This methodology will be applied in a case study at a P&P mill. This P&P mill aims to implement the FBR by producing bioproducts. After market analysis and LBA, two product/process portfolios are considered, which are shown in Table 2.

Table 2. Price change scenarios

Product/Process portfolio No.1	Product/Process portfolio No.2
P1 (2000 tonne/day)	P3 (500 tonne/day)
P2 (1000 tonne/day)	P4 (350 tonne/day)

In the next step the range of required flexibility must be determined. Three price scenarios are generated for each portfolio, as shown in Table 3.

Table 3. Price change scenarios

	Pessimistic	Likely	Optimistic
P1	\$1.50/gal	\$3.00/gal	\$3.50/gal
P2	\$350/tonne	\$485/tonne	\$600/tonne
P3	\$1500/tonne	\$1900/tonne	\$2100/tonne
P4	\$3000/tonne	\$3300/tonne	\$3500/tonne

The first and third scenarios consider price decrease and increase for all products, respectively, while the second scenario represents the most probable case in the market. For each of these scenarios, the developed SC model is run without constraint on production capacity in order to obtain the optimal production rate of each process for each scenario, and to determine the production range as the flexibility measure. Table 4 shows the production rate needed for each process in the case of each scenario realization.

Table 4. Production rate for each process in the case of scenario realization

	Pessimistic	Likely	Optimistic
P1	1200 t/d	2000 t/d	2100 t/d
P2	700 t/d	1000 t/d	1050 t/d
P3	400 t/d	500 t/d	510 t/d
P4	300 t/d	350 t/d	350 t/d

Therefore, -40%, -30%, -20% and -14% of flexibility are the maximum flexibility needed for P1, P2, P3 and P4 production processes, respectively. In the next step design alternatives are defined based on calculated ranges of flexibility.

The manufacturing processes in both portfolios are characterized as:

- Lines in series

- Each line produces only one product

The manufacturing system for each portfolio is illustrated in Figure 8.

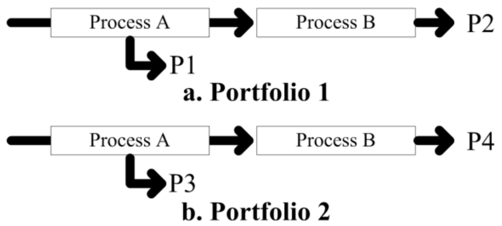

Figure 8. Process schematic for portfolio a) 1, b) 2

As none of the processes can handle the obtained levels of flexibility, therefore the production lines must be divided into 2 or more lines whose sum of production rates is equal to the nominal rate, e.g. 2000 tons/day of P1. For each process, two alternatives have been considered. Given that the nominal production rate for P1 and P2 is 2000 tons/day and 1000 tons/day, respectively, design alternatives for the first portfolio are illustrated in figure 9. The design alternatives are defined as presented in Table 5.

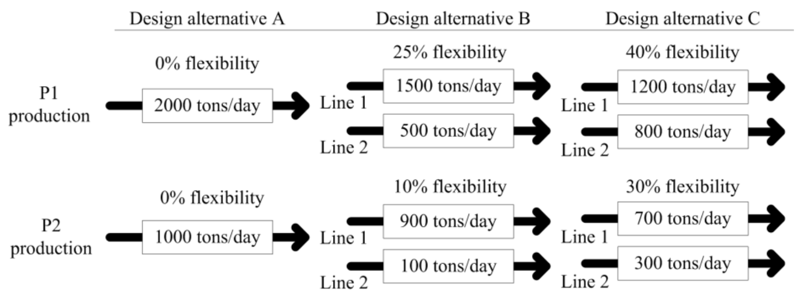

Figure 9. Design alternatives for the first portfolio

Table 5. Design alternatives for each portfolio

Design case	**Portfolio 1: Etoh/Ethylene**			**Portfolio 2: LA/PLA**		
	Design Alter.	Mfg. Flex.	Cap. Inv.	Design Alter.	Mfg. Flex.	Cap. Inv.
Base Case Design	A-P1	0%	$180M	D- P3	0%	$100M
	A- P2	0%	$70M	D-P4	0%	$80M
Flexible Design 1	B- P1	25%	$203M	E- P3	10%	$107M
	B- P2	10%	$75M	E-P4	10%	$86M
Flexible Design 2	C- P1	40%	$206M	F- P3	20%	$111M
	C- P2	30%	$79M	F-P4	14%	$88M

Then normalized SC profit for each portfolio in the case of all scenario realizations is calculated for all design alternatives. The results are shown in Table 6.

Table 6. Normalized SC profit

Portfolio	Price Scenarios	Assumed Mfg Flexibility		
		0%	**25%**	**40%**
P1/P2	Pessimistic	0.3	0.7	0.9
	Likely	1	1.1	1.15
	Optimistic	1.05	1.15	1.2
		0%	**10%**	**30%**
P3/P4	Pessimistic	-0.5	-0.2	-0.05
	Likely	1	1	1
	Optimistic	1.01	1.05	1.1

Based on the SC profit and capital investment required for each design alternative, the ROI can be estimated for all design alternatives and price scenarios. Figure 10 illustrates the ROI of each design alternative for each price scenario.

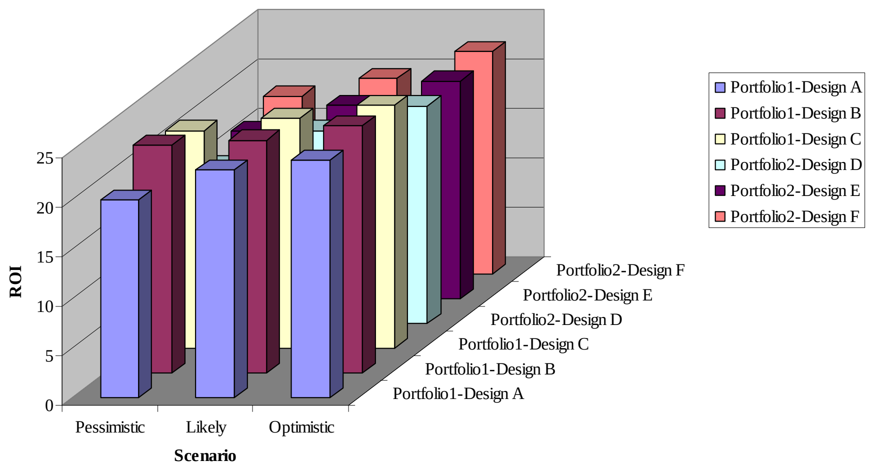

Figure 10. ROI of design alternatives for each price scenario

According to the resulting ROIs, design B for the first portfolio and design F for the second portfolio are better choices.

For the next step, which deals with SC network design, two SC network alternatives are defined for each of these design alternatives in terms of establishing a new warehouse and expanding the existing warehouse. The SC model is employed to calculate the profitability of these SC network alternatives for each portfolio and to find the best network option. The results are shown in Table 7.

Table 7. SC profit for each network alternatives

	Etoh/Ethylene (Design B)			LA/PLA (Design C)		
SC Design	Base case	Sc 1	Sc 2	Base Case	Sc 1	Sc 2
Pess.	0.79	0.87	0.92	0.7	0.94	0.9
Likely	1	1.1	1.2	0.95	1.02	1.01
Opti.	1.13	1.18	1.24	1.01	1.09	1.05

Finally, SC profitability, range of flexibility and ROI will be used as SC metrics in a multi-criteria decision making framework in order to determine the best set of product/process portfolios from a specific company point of view. It must be mentioned that such complex problems are combinatorial. If the feedbacks from later stages to the earlier ones are not considered, some opportunities might be missed. But as mentioned in the introduction, this hierarchical methodology aims to find an improved business model by addressing market strategies, emerging products/processes, and the manufacturing flexibility required for mitigating market uncertainty, and does not seek the best option. Scenarios that are made at each step for product/process portfolio, design alternatives representing different levels of flexibility, and SC network alternatives are all generated by experts who consider the major aspects of the problem. Hence, the crucial issues that must be considered in defining biorefinery strategies will be reflected at each step to ensure identifying a set of feasible and practical options. But in some cases, considering the feedback, especially from the third step to the second step, might be necessary. This necessity arises from the impacts of SC network alternatives on the flexibility design alternatives. Defined network scenarios might change the flexibility needed for mitigating market risks. In this way, this methodology will help experts to identify possible options for further decision making steps.

6. Conclusions

A hierarchical methodology is proposed to integrate product/process portfolio design, design of manufacturing flexibility, and SC network design. Market analysis, SC optimization and techno-economic study are employed as tools. Scenario generation is used to address the product price and demand volatility. Inspired by work done previously in Environmental Design Engineering Chair at Ecole Polytechnique in Montréal regarding SC-based analysis in the context of P&P

industry, this methodology shows how the FBR can be implemented strategically via a step-wise approach. Through this step-wise approach, different options in terms of product/process portfolio can be studied and their potential for manufacturing flexibility can be investigated. Also, the best SC network for these options can be identified. Therefore product portfolio design and process design can be reflected in the SC strategic design via this SC-based analysis. The result of this analysis enables systematic consideration of the SC profit at the early-stage design for different product/process portfolios.

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APPENDIX B - Article: Metrics for evaluating the forest biorefinery supply chain performance

Metrics for Evaluating the Forest Biorefinery Supply Chain Performance

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Abstract

The forest biorefinery (FBR) is emerging as a possibility for improving the business model of forest product companies, however introduces significant challenges in terms of market, technological, and financial risks - which can be addressed to an important extent in the design of supply chains (SC). For sustainable decision-making regarding biorefinery strategies, criteria from different perspectives, i.e. economic, environmental and social, should be considered. The economic criteria that are used for decision making typically do not consider volatility, whereas today's market is subject to volatilities in terms of price and demand. It is critical that biorefinery strategies are flexible in order to be robust to market volatility. This paper presents metrics of flexibility and robustness, showing the performance of the SC in a dynamic environment. These metrics are suitable to be used in a multi-criteria decision-making (MCDM) framework for the evaluation of the FBR SC strategies. Moreover, a "conditional value-at-risk" parameter is introduced for analyzing levels of risks in making sales decisions.

Keywords: Forest Biorefinery, Supply Chain, Flexibility, Robustness, Value-at-risk

1. Introduction

FBR is increasingly considered as a possibility for improving the forest products company business model, though it poses market, technological, and financial challenges. Thus, potential FBR implementation strategies must be analyzed using different perspectives to identify the most promising ones. Sustainable development includes three dimensions; economic, environmental, and social (Janssen, Chambost & Stuart, 2009). For a strategy to be sustainable, it must have good performance in all three dimensions. MCDM frameworks can consider several metrics

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provided from different analysis tools to permit the analysis of different strategies (Janssen, Chambost & Stuart, 2009). Hence, MCDMs can be used for sustainability analysis, if appropriate metrics for economic, environmental and social aspects of a strategy can be assessed.

Integrating different tools for analyzing product/process strategies is gaining attention. One of the first efforts was done by Zhou, Cheng and Hua (2000) who described a goal programming approach in order to consider the sustainability aspects of continuous process industries' supply chain. Hugo and Pistikopoulos (2005) proposed the combination of life cycle assessment criteria with design and long-range planning of multi-enterprise supply chain networks. Sammons, Eden, Yuan, Cullinan and Aksoy (2007) proposed a general systematic framework including SC optimization for optimizing product portfolio and process configuration in integrated biorefineries. Guillén-Gosálbez and Grossmann (2010) addressed the optimal design and planning of sustainable chemical supply chains using a bi-criterion stochastic non-convex mixed-integer nonlinear program which accounts for both net present value (NPV), and environmental performance of the network through Eco-indicator 99, which included recent advances made in life cycle assessment (LCA). Mansoornejad, Chambost and Stuart (2010) introduced a systematic hierarchical methodology to integrate product portfolio design with SC network design in the FBR. Separate methodologies for product portfolio definition, process technology selection, and SC design are integrated in the proposed hierarchical methodology. Sharma, Sarker and Romagnoli (2011) introduced a model for assessing the impact of feedstock and technology selection, process and utility integration, and effluent recycle for a multi product multi platform biorefining enterprise. Cisneros, Grau, Anton, Prada, Cantero and Degioanni (2011) used three continuous multi-criteria approaches and a set of different weights to assess the conflicts and trade-off among environmental, economic and social interests in the context of agriculture (soybean production). Mele, Kostin, Guillen-Gosalbez and Jimenez (2011) developed a multiobjective mixed-integer linear program that is used as a quantitative tool to support SC design decision-making and aims at optimizing the economic and environmental performance of a combined sugar and ethanol production chain.

As mentioned earlier, several metrics from different tools are required for quantifying the performance of a strategy from different perspectives. Economic metrics that are used in decision making, which are mainly related to the profitability of a strategy, are incapable of accounting for the market volatility (Hytonen & Stuart, 2011). Sensitivity analysis is typically executed to address the impact of possible market scenarios on profitability. Even in this case, the problem is viewed as a steady-state case and the dynamism of the market, i.e. changes in price and demand over the given time period, are ignored. Moreover, it is not easy to use the result of a sensitivity analysis in an MCDM framework. Instead, it is desirable to reflect the response of a strategy to such dynamism by relevant metrics. This paper presents metrics of flexibility and robustness that can be used in an MCDM framework, in conjunction with economic criteria, for the evaluation of the FBR process options and SC strategies. These metrics are the outcomes of an analysis performed by an SC optimization framework that evaluates the impacts of the SC design on operational SC activities. Moreover, a conditional value-at-risk parameter is introduced to analyze levels of risk in making sales decisions and to provide required information for profit-risk trade-offs. The remainder of this article is organized as follows; first, the problem statement is described. Next, the performance metrics are explained. Then, the SC optimization framework is presented and the case study is introduced. Afterwards, the application of each metric is illustrated. Finally, the general and concluding remarks of the work are drawn.

2. Problem statement

The decision as to what biorefinery strategy to take depends on many factors, most of which cannot be reflected in an optimization problem, e.g., understanding the market and market strategies, emerging products and technologies, the capabilities of existing SC assets, and potential partners. In a practical problem, it is difficult to address all these decisions within a single SC optimization model. Instead, it is preferable to pursue a systematic hierarchical methodology that addresses all these factors in a stepwise manner. Because of the combinatorial aspect of such design problems, the hierarchical methodology might miss the global optimum. However, this hierarchical methodology does not seek to identify a global optimum. Rather, it seeks a set of feasible and practical biorefinery options that a company can strategically pursue. Many of the key aspects can be addressed by defining different scenarios and options/alternatives instead of being modelled into an optimization formulation. In this way, a simpler model will be solved, with more practical results. This methodology would end up with a set of solutions. A multi-criteria decision-making (MCDM) framework can be used to find the best option from a specific company's point of view (Mansoornejad, Chambost, & Stuart, 2010).

Major strategic SC decisions addressed by a forest product company implementing the FBR include which products to produce, which technologies to employ, with which companies to make partnerships, and which parts of the SC to redesign. The SC of an FBR must be designed to be flexible, so that it can have a robust response to market volatility. The goal of this paper is to propose appropriate metrics to quantify flexibility and robustness in order to evaluate the performance of several FBR design options. These metrics can be used in designing flexible and robust systems, e.g. in targeting the flexibility of a system at the design stage. Moreover, such metrics can be utilized in comparing different design options. Design options with different levels of flexibility in production and with different SC networks are considered, and their performance in case of several market scenarios is tested. An SC optimization model calculates the profit of design options for every market scenario and quantifies the flexibility and robustness of each option using the introduced metrics. These metrics can be further used in an MCDM framework along with metrics provided by other tools, e.g. life cycle analysis (LCA), to identify the best option.

Fig. 1 shows how several metrics can be used in an MCDM framework (Mansoornejad, Chambost, & Stuart, 2010). Market-based analysis, which involves a product portfolio definition/selection methodology, is used to identify a set of viable product portfolios. For an FBR, each product portfolio comprises a number of products, including existing pulp and paper products and new bioproducts. After this step, several methodologies are applied to provide the appropriate metrics. Techno-economic study can provide economic metrics such as Internal Rate of Return (IRR), while LCA can generate several metrics related to environmental aspects of implementing each option. This paper focuses on the SC analysis. Given is a set of product portfolios, a set of process technologies that can be used to produce those products with known capital and operating cost, and the configuration of the SC network. Several market scenarios, including product price and demand change over a period of one year, are also defined as the input to the problem to represent market volatility. The model is run for a time horizon of one year divided into 48 weeks as time periods. An SC model, which is presented in the paper, is used as a tool in the SC analysis. The output of the analysis is SC-related metrics, i.e. SC profitability, robustness (of profitability), and flexibility, to be used by the MCDM framework.

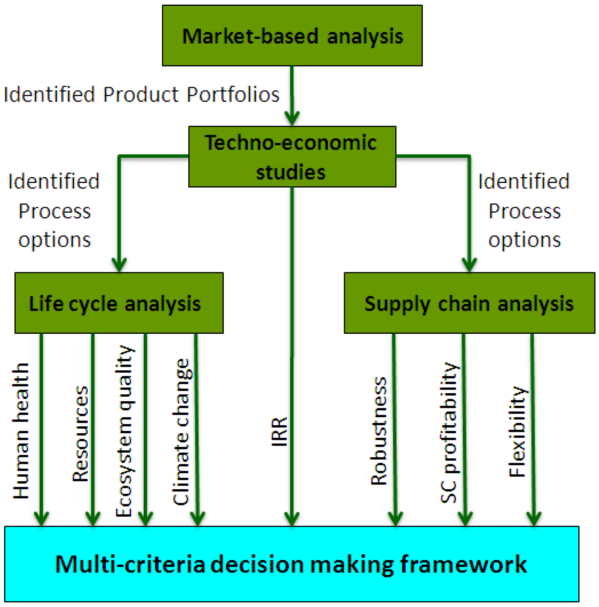

Fig. 1. MCDM framework

3. Performance metrics

As stated by Beamon (1998), establishment of appropriate performance measures is an important component in supply chain design and analysis. Performance measures can be used either in comparing competing alternative systems, or in designing proposed systems, by determining the values of the decision variables that yield the most desirable level(s) of performance. These measures can be classified into two categories; qualitative and quantitative. Qualitative performance measures are those measures for which there is no single direct numerical measurement, although some aspects of them may be quantified. Customer satisfaction, flexibility, information and material flow integration, effective risk management, supplier performance are example of qualitative measures. On the other hand, quantitative performance measures may be defined numerically. Such measures may be described by, either objectives that are based directly on cost or profit such as cost minimization, sales maximization, profit maximization, inventory investment minimization, return on investment maximization, or objectives that are based on some measure of customer responsiveness like fill rate maximization, product lateness minimization, customer response time minimization, lead time minimization, function duplication minimization.

Beamon defined the measure of flexibility as the degree to which the supply chain can respond to random fluctuations in the demand pattern. This is a generic definition and involves all types of flexibility. In this paper, we try to present a metric of flexibility that can be well applied for design purposes for the FBR design. Moreover, as mentioned earlier, it is important to be able to reflect market volatility in the decision making and to evaluate the performance of an SC in such an environment. In other words, the robustness of SC against different market conditions needs to be quantified. Some metrics were defined for this purpose, which will be discussed further in this section of the paper.

3.1. *Manufacturing flexibility: Metric of flexibility (MF)*

Today's market is subject to huge volatilities in terms of price and demand. The price of oil, fuels, and chemicals, as well as the price of forestry products, change even on a monthly basis. The demand for some products is not always certain, and sometimes, despite strong demand, the price is too low for the production of a product to be profitable. On the feedstock side, uncertainty exists in terms of price and availability. A forestry company might be obliged to procure its feedstock from different sources over different distances and with different prices. Short product life cycles and increasing competition among companies reveal new uncertainties and risks for different industries. All these clauses entail more uncertainty and risk for the companies. To mitigate risks in the face of such uncertainties, it is of crucial importance to enhance adaptiveness and reactivity on one hand and proactivity on the other hand (Schiltknecht, & Reimann, 2009). These capabilities are generally called flexibility. Based on the type of uncertainty and how it is addressed, there are different types of flexibility.

An FBR will be exposed to this kind of volatile environment and will face these risks and uncertainties. Hence, flexibility, of any possible type, must be exploited in an FBR to mitigate risks. An FBR will be able to produce several products, including P&P products, bioproducts, and energy. Producing several products implies the opportunity to take advantage of manufacturing flexibility, i.e., producing different products at different volumes in different time periods. In a volatile market, depending on feedstock and product prices as well as supply and demand, manufacturing flexibility can be exploited, and the mill can produce different products in different amounts to optimize and secure the company's margin. The company should analyze its access to feedstock, product prices, and received as well as forecasted demands and find the best alignment between these demands and its production capacity to maximize the company's profit.

The concept of manufacturing flexibility in the FBR implies the ability to produce several bioproducts (product flexibility) at different volumes (volume flexibility) and in different time periods based on product price and demand. This definition is an aggregation of product flexibility and volume flexibility. Manufacturing flexibility implies a justifiable increase in capital cost that is adequately compensated by the ability of the process to manufacture in a flexible manner so that the expected volatility in market conditions can be mitigated.

In the design of chemical processes, volume flexibility has a critical role. Thus, in order to design or analyse the flexibility of a system, quantifying volume flexibility is of crucial importance. Inspired by the work of Voudouris (1996) on qualitative measure of flexibility, metric of flexibility (MF) quantifies volume flexibility, as shown in equation 1:

$$MF = \sum_t \sum_p \sum_m \left| \frac{C_{mpt} - C_{mp}^N}{C_{mp}^N} \right| \quad (1)$$

where $\boldsymbol{C_{mpt}}$ is the amount of product *m* that is produced on process *p* in time period *t* and $\boldsymbol{C_{mp}^N}$ is the amount of product *m* produced on process *p* by the nominal production rate over the same number of processing hours. This formulation shows the deviation from the nominal production rate in a dimensionless form and implies volume flexibility.

3.2. *Robustness: Metric of robustness (MR)*

In a robust design the control parameters of a system are selected in such a way that the desirable measured function do not diverge significantly from a given value (Bernardo, Pistikopoulos, & Saraiva, 1999). In this work, robustness is not considered in the optimization formulation. Instead, a metric of robustness (MF) is used to quantify the robustness of design options against market volatility so that design options can be compared in terms of robustness. Several robustness metrics have been introduced thus far (Vin & Ierapetritou, 2001). Well-known metrics are standard deviation and mean absolute deviation (Bernardo, Pistikopoulos, & Saraiva, 2001). For the sake of simplicity and interpretability for an MCDM panel, we use a simple formulation as robustness metric, as shown in equation 2.

$$MR = \left(\frac{\sum_{Sc} (Pr_B - Pr_{Sc})}{Pr_B} \right)^{-1} \qquad (2)$$

where $\mathrm{Pr_B}$ is the base case profit, $\mathrm{Pr_{Sc}}$ is the profit for scenario Sc and $\mathrm{N_{Sc}}$ is the number of scenarios. In this work, the desired parameter that must not diverge from a given value is profit. It is desirable that the profit of a design option in case of each market scenario does not deviate from the base case profit, if this profit is lower than the base case profit. Therefore, to quantify the downside risk of volatility, calculated profits that are less than the base case profit are considered in this equation. The MR shows the percentage of aggregate deviation from the base case profit for all profits less than the base case profit. The smaller this percentage is the better and more robust the system is. Hence, we use the reverse of the percentage, so that the higher values of MR represent more robust systems.

4. SC optimization framework

Fig. 2 illustrates the SC of an FBR. Several types of feedstock, ranging from forest biomass to recycled papers and agricultural residues, can be used. Feedstock is treated and prepared to be used in the plants. The final products involve wood and paper products, biofuel, green chemicals and energy.

The SC framework presented in this paper aims at maximizing profit across the entire SC by identifying the tradeoffs between demand and production capabilities, and by finding the optimal alignment of manufacturing capacity and market demand. The SC optimization framework considers feedstock price and availability, production costs, and inventory and delivery costs, as well as product price and demand. Taking this information into account, the SC optimization framework will exploit the potential for flexibility and determine which orders must be fulfilled, and therefore, how much of which products must be produced, how they should be stored, and how they should be delivered to the market to maximize SC profit.

There is a strong body of knowledge related to SC mathematical formulation. Such formulations address strategic design, tactical planning or operational and scheduling SC decisions. Some examples can be viewed in Voudouris (1996), Timpe and Kallrath (2000), Jin-Kwang, Grossmann, and Park (2000), Tsiakis, Shah, and Pantelides (2001), Sousa, Shah, and Papageorgiou (2005), and You and Grossmann (2008). Some formulations integrate these decisions and combine strategic decisions with tactical ones or tactical decisions with operational ones, in order to reflect the effect of lower level decisions into higher levels. Instances of such formulations can be found in Sabri and Beamon (2000), Kallrath (2002), Sousa, Shah, and Papageorgiou (2008), Maravelias and Sung (2009), and Shah and Ierapetritou (2011).

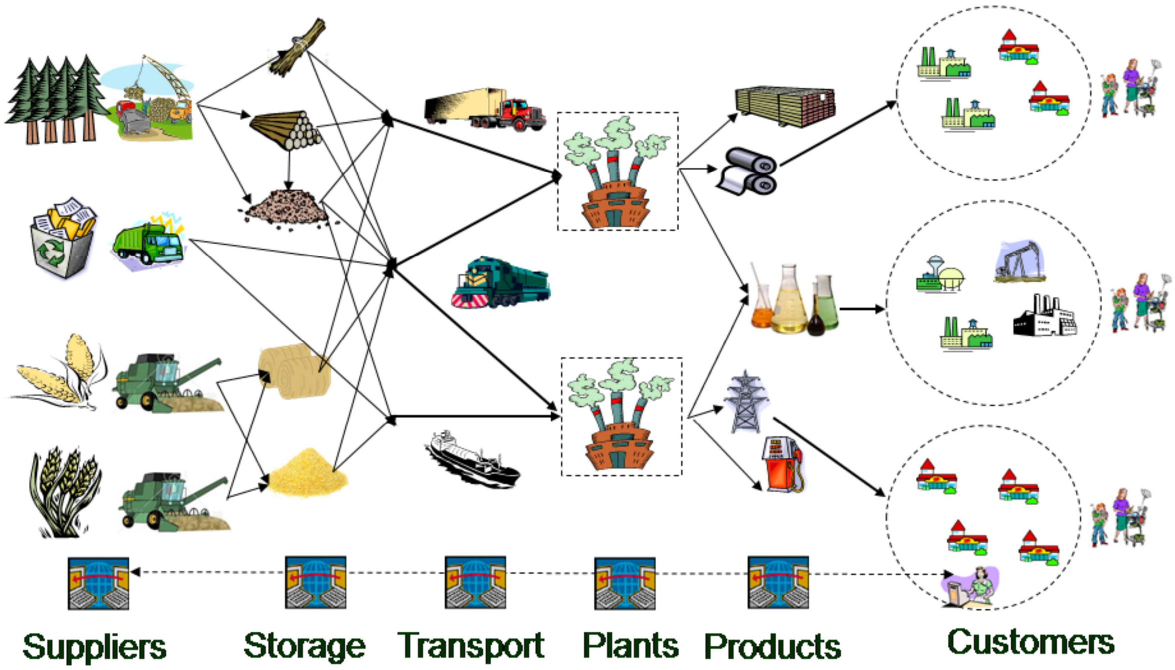

Fig. 2. Forest biorefinery supply chain

It is desirable to account for tactical and operational issues at the strategic design level. On the other hand, for design purposes, it is not necessary to go down to too much details, as provided by scheduling models. For this reason, the SC framework that is presented in this work is inspired by the tactical model developed for the chemical industry by Kanegiesser (2008). This model is a tactical model that has some operational components. The model divides each time period into several hours that can be dedicated to production, changeover or maintenance. In this way, a better cost representation can be made by the model.

The framework is formulated as an optimization problem with the objective of maximizing profit. This framework considers the management of a multi-product, multi-echelon SC, including existing production and warehousing facilities as well as a number of customer zones, although it can also be used for design purposes. Different types of biomass are provided by several suppliers. Production facilities can make one or several products. Processes are either dedicated, i.e. they produce only one product, or flexible from a product perspective, i.e. they are able to produce several products through different production modes or "recipes". In other words, a flexible process can use different recipes to produce different products. Changing from one recipe to another incurs changeover cost and time. Processes can be idled or shutdown for scheduled maintenance. The steam required for each process is provided by both fuel and biomass. Warehouses can receive material, either feedstock or product, from different sources and plants, and supply different markets. Each market places demand in two ways: by contract, i.e., for the long term, and on the spot market, i.e., for the short term. In case of a contract, specific quantities of products must be sold to the customer in specific time periods. The spot demand can be partially fulfilled. Transportation routes link suppliers, facilities and customers together. The model is formulated as a mixed integer linear programming (MILP) problem with a discrete time horizon of 48 weeks. Each time period is broken down into hours. Several subsets have been created to link parameters and variables to each other. For instance, processes can only produce certain materials. This will reduce the possible options and thus, the complexity of the problem. It is worth noting that the metrics are neither used in any of the model constraints nor they are optimized. They are just calculated after the model is run. The model is presented below:

Nomenclature

Sets

$j \in J$	Supplier locations
$l \in L$	Mill locations
$k \in K$	Sales locations
$p \in P$	Processes
$r \in R$	Recipes
$m \in M$	Materials
$t \in T$	Time

Subsets

Suppliers that can supply mill: $\{j,l\} \in L^{JL} \quad \forall j \in J, l \in L$

Customers that can be served by mill $\{l,k\} \in L^{LK} \quad \forall l \in L, k \in K$

Processes at mill $\{l,p\} \in P^{L} \quad \forall l \in L, p \in P$

Recipes available on process $\{l,p,r\} \in R^{P} \quad \forall\{l,p\} \in P^{L}, r \in R$

Materials offered by suppliers $\{j,m\} \in M^{J} \quad \forall j \in J, m \in M$

Materials produced/processed at mill $\{l,m\} \in M^{L} \quad \forall l \in L, m \in M$

Materials requested by customers $\{k,m\} \in M^{K} \quad \forall k \in K, m \in M$

Input materials of a process $\{l,p,m\} \in M^{P-in} \quad \forall\{l,p\} \in P^{L}, m \in M$

Output materials of a process $\{l,p,m\} \in M^{P-out} \quad \forall\{l,p\} \in P^{L}, m \in M$

Input materials of a recipe $\{l,p,r,m\} \in M^{R-in} \quad \forall\{l,p,r\} \in R^{P}, m \in M$

Output materials of a recipe $\{l,p,r,m\} \in M^{R-out} \quad \forall\{l,p,r\} \in R^{P}, m \in M$

Constructed Subsets

Materials that can be transported between a supplier and a mill:

$\{j,l,m\} \in M^{JL} \quad \forall\{j,l\} \in L^{JL}, \{j,m\} \in M^{J}, \{l,m\} \in M^{L}$

Materials that can be transported between a mill and a customer:

$\{l,k,m\} \in M^{LK} \quad \forall\{l,k\} \in L^{LK}, \{l,m\} \in M^{L}, \{k,m\} \in M^{K}$

Parameters

a_{lprm}^{input}	Recipe material conversion Input factor of material m when using recipe r on process *p* in mill *l* (dependent on throughput)
a_{lprm}^{output}	Output factor of material *m* when using recipe *r* on process *p* in mill *l*
$b_{lpr}^{input-steam}$	Steam consumption factor for recipe *r* in process *p* in mill *l*
$b_{lpr}^{output-steam}$	Steam production factor for recipe *r* in process *p* in mill *l*
$b_{lpr}^{input-elect}$	Electricity consumption factor for recipe *r* in process *p* in mill *l*
$b_{lpr}^{output-elect}$	Electricity production factor for recipe *r* in process *p* in mill *l*

$c_{lpr}^{proc-var}$	Variable operating cost of using recipe r on process p in mill l (dependent on process throughput)
$c_{lt}^{mill-fix}$	Fixed operating cost at mill *l* during time period *t*
$c_{jlm}^{transport-sup}$	Transportation cost of material *m* from supplier *j* to mill *l*
$c_{lkm}^{transport-sales}$	Transportation cost of material *m* from mill *l* to a customer *k*
c_{lm}^{stor}	Storage cost of material *m* in mill *l*
$c_{lp}^{shutdown}$	Shutdown cost of process *p* in mill *l*
$c_{lp}^{changeover}$	Changeover cost of process *p* in mill *l*
c_{lt}^{elect}	Electricity cost / selling price at mill *l* during time period *t*
c_{kmt}^{sales}	Selling price of product *m* to customer *k* during time period *t*
c_{jmt}^{sup}	Purchasing price of a feedstock *m* from supplier *j* during time period *t*
$c_{kmt}^{salescost}$	Sales cost for product *m* sold to customer *k* during time period *t*
H_{lpr}^{camp}	Minimum campaign length for recipe *r* in process *p* in mill *l*
$H_{lp}^{changeover}$	Changeover time on process *p* in mill *l*
H_{lpt}^{proc}	Available processing hours on process *p* in mill *l* during time period *t*
$\underline{Q}_{lpr}^{proc}$	Minimum throughput (process rate) of recipe *r* on process *p* in mill *l*
$\overline{Q}_{lpr}^{proc}$	Maximum throughput (process rate) of recipe *r* on process *p* in mill *l*
$\underline{Q}_{lm}^{stor}$	Minimum storage quantity of material *m* in mill *l*
$\overline{Q}_{lm}^{stor}$	Maximum storage quantity of material *m* in mill *l*
$\underline{Q}_{jmt}^{supp}$	Minimum supply quantity of material *m* offered by supplier *j* during time period *t*
$\overline{Q}_{jmt}^{supp}$	Maximum supply quantity of material *m* offered by supplier *j* during time period *t*
$\underline{Q}_{kmt}^{sales}$	Minimum quantity of material *m* requested by customer *k* during time period *t*
$\overline{Q}_{kmt}^{sales}$	Maximum quantity of material *m* requested by customer *k* during time period *t*
$\overline{Q}_{jlm}^{transport}$	Maximum transportation quantity of material *m* between supplier *j* and mill *l*
$\overline{Q}_{lkm}^{transport}$	Maximum transportation quantity of material *m* between customer *k* and mill *l*

$S_{lm}^{mat-start}$	Initial storage quantity of material *m* in mill *l* at time 0
$S_{lm}^{mat-end}$	Minimum storage quantity of material *m* in mill *l* at time T
ε_{lpt}^{proc}	Shutdown hours on process *p* in mill *l* during time period *t*
$\alpha_{lpr}^{rec-start}$	Initial recipe *r* on process *p* in mill *l*

Variables

f_{jlmt}^{sup}	Flow of material *m* from supplier *j* to mill *l* during time period *t*
f_{lkmt}^{mill}	Flow of material *m* from mill *l* to customer *k* during time period *t*
h_{lprt}^{rec}	Number of hours spent on recipe *r* on process *p* in mill *l* during time period *t*
S_{lmt}^{mat}	Inventory of material *m* in mill *l* during time period *t*
v_{lpt}^{input}	Input steam quantity on process *p* in mill *l* during time period *t*
v_{lpt}^{output}	Output steam quantity on process *p* in mill *l* during time period *t*
w_{lpt}^{input}	Input electricity quantity on process *p* in mill *l* during time period *t*
w_{lpt}^{output}	Output electricity quantity on process *p* in mill *l* during time period *t*
x_{lmpt}^{proc}	Input quantity of material m on process *p* in mill *l* during time period *t*
y_{lmpt}^{proc}	Output quantity of material m on process *p* in mill *l* during time period *t*
y_{lprmt}^{rec}	Output quantity of material m using recipe *r* on process *p* in mill *l* during time period *t*
$y_{lprt}^{rec-tot}$	Total mass output of recipe *r* on process *p* in mill *l* during time period *t*
α_{lprt}^{proc}	Selection of recipe *r* on process *p* in mill *l* during time period *t* (binary)
β_{lprt}^{proc}	Successive selection of recipe *r* on process *p* in mill *l* during time periods *t* and *t-1* (binary)
θ_{kmt}^{ord}	Selection of the order of product *m* from customer *k* during time period *t* (binary)

Objective Function

The objective function is the global net profit of the enterprise to be maximized. This profit consists of revenues from the sales of products and electricity, minus several variable and fixed costs.

$$\max Profit = \begin{pmatrix} Revenues - ElectricityCost - SalesCost \\ -VariableOpCost - FixedOpCost - ChangeoverCost - ShutdownCost \\ -TransportationCost - StorageCost - ProcurementCost \end{pmatrix}$$

(3)

Revenues from sales are equal to the flow of materials sent to each customer multiplied by the selling price.

$$Revenue = \sum_{t\in T} \sum_{\{k,m\}\in M^K} f_{lkmt}^{sales} c_{kmt}^{sales} \quad (4)$$

Electricity sales or purchases are function of the production/consumption at the mill. If the mill produces more electricity than needed, then electricity is sold to the grid. Otherwise, it is assumed it is bought from the grid at the same price.

$$ElectricityCost = \sum_{t\in T} \sum_{\{l,p\}\in P^L} (w_{lpt}^{input} - w_{lpt}^{output}) c_{lt}^{elect} \quad (5)$$

Variable sales costs are customer specific and are a percentage of product prices.

$$SalesCost = \sum_{t\in T} \sum_{\{k,m\}\in M^K} f_{lkmt}^{sales} c_{kmt}^{salescost} \quad (6)$$

Variable operating costs are a function of process throughput such as chemical consumption.

$$VariableOpCost = \sum_{t\in T} \sum_{\{l,p,r\}\in R^P} c_{lpr}^{proc-var} y_{lprt}^{rec-total} \quad (7)$$

Fixed operating costs are calculated at the plant.

$$FixedOpCost = \sum_{t\in T} \sum_{l\in L^{mill}} c_{lt}^{mill-fix} \quad (8)$$

Changeover cost is equal to the number of transitions multiplied by the changeover cost per transition. This cost is not considered sequence dependent.

$$ChangeoverCost = \sum_{t\in T} \sum_{\{l,p,r\}\in R^P} (1 - \sum_{r\in R_p^{proc}} \beta_{lprt}^{proc}) \, c_{lp}^{changeover} \quad (9)$$

The shutdown cost of a process is a function of the number of shutdown hours during a time period. Scheduled shutdowns for maintenance are considered here as a hard constraint.

$$ShutdownCost = \sum_{t\in T} \sum_{\{l,p\}\in P^L} \varepsilon_{pt}^{proc} c_{lp}^{shutdown} \quad (10)$$

Transportation cost is calculated by multiplying the amount of material shipped from a source (supplier *j* or mill l) to a sink (mill *l* or customer *k*) and the shipping cost per mass of that route.

$$TransportationCost =$$

$$\sum_{t\in T}\sum_{\{j,l,m\}\in M^{JL}} f_{jlmt}^{sup} c_{jlm}^{transport-sup} + \sum_{t\in T}\sum_{\{l,k,m\}\in M^{LK}} f_{klmt}^{sales} c_{jlm}^{transport-sales} \quad (11)$$

Storage cost in a facility is equal to the amount of material kept in inventory during each time period multiplied by its storage cost per month.

$$StorageCost = \sum_{t\in T}\sum_{\{m,l\}\in M^{L}} S_{mlt}^{mat} c_{lm}^{stor} \quad (12)$$

Procurement costs are equal to the flow of materials transported from each supplier to different facilities multiplied by the selling price.

$$ProcurementCost = \sum_{t\in T}\sum_{\{j,l,m\}\in M^{JL}} f_{ll'mt}^{sup} c_{lmt}^{sup} \quad (13)$$

Demand and Procurement

Suppliers and customers may offer/request materials between lower and upper fulfilment bounds, as shown in equations 14 and 15. Lower and upper bounds for customers are multiplied by binary variable θ, which is equal to one if the order is fulfilled and equal to zero otherwise. For contractual orders, the lower and upper bounds are equal, because the contractual amount is fixed. But the lower bound for spot orders is equal to zero and the model can determine what percentage of the order should be fulfilled. Equation 16 forces θ of all time periods to be equal to θ of first time period. In this way, if an order is accepted in the first period, it must be fulfilled over all other time periods. This constrain refers to contractual orders, which either must be fulfilled throughout the year, or must be refused. This will not cause any problem for spot orders, which can be fulfilled partially at any time, because if model decides not to fulfil a spot order, model can assign zero to fulfilled amount for this order, as the lower bound for spot order fulfilment is zero, no matter if θ is zero or one. Thus, it can be said that θ is one for all spot orders and can be zero or one for contractual orders.

$$\underline{Q}_{lmt}^{supp} \leq f_{ll'mt}^{sup} \leq \overline{Q}_{lmt}^{supp} \qquad \forall\ \{j,l,m\} \in M^{LJ}, t \in T \quad (14)$$

$$\theta_{ll'mt}^{ord}\underline{Q}_{lmt}^{sales} \leq f_{l'lmt}^{sales} \leq \theta_{ll'mt}^{ord}\overline{Q}_{lmt}^{sales} \qquad \forall\ \{l,k,m\} \in M^{LK}, t \in T \quad (15)$$

$$\theta_{ll'm1}^{ord} = \theta_{ll'mt}^{ord} \qquad \forall\ \{l,k,m\} \in M^{LK}, t > 1 \quad (16)$$

Transportation

A maximum transportation capacity constraint limits the amount of materials that can be transported between locations (suppliers, facilities and customers).

$$f_{jlmt}^{sup} \leq \overline{Q}_{jlm}^{transport-sup} \qquad \forall \ \{j,l,m\} \in M^{LJ}, t \in T \tag{17}$$

$$f_{lkmt}^{mill} \leq \overline{Q}_{lkm}^{transport-sales} \qquad \forall \ \{l,k,m\} \in M^{LK}, t \in T \tag{18}$$

Inventory Management

The material balance at a facility is equal to the previous inventory, plus/minus material coming from and going to other sites as well as the consumption/production from processes.

$$S_{mlt}^{mat} = S_{mlt-1}^{mat} + \sum_{\{j,l,m\} \in M^{JL}} f_{jlmt}^{sup} - \sum_{\{l,k,m\} \in M^{LK}} f_{lkmt}^{sales} + \sum_{\{l,l',m\} \in M^{LL}} f_{ml'lt}^{mill} - \sum_{\{l,l',m\} \in M^{LL}} f_{mll't}^{mill} - \sum_{\{l,p,m\} \in M^{P-out}} x_{lmpt}^{proc} + \sum_{\{l,p,m\} \in M^{P-in}} y_{lmpt}^{proc} \qquad \forall \{l,m\} \in M^{L}, t > 1 \tag{19}$$

At time t=1, S_{mlt-1}^{mat} does not exist and it is replaced by the initial inventory quantity, S_{ml}^{start}.

$$S_{ml1}^{mat} = S_{ml}^{start} + \sum_{\{j,l,m\} \in M^{JL}} f_{jlm1}^{sup} - \sum_{\{l,k,m\} \in M^{LK}} f_{lkm1}^{sales} + \sum_{\{l,l',m\} \in M^{LL}} f_{ml'l1}^{mill} - \sum_{\{l,l',m\} \in M^{LL}} f_{mll'1}^{mill} - \sum_{\{l,p,m \in M^{P-out}\}} x_{lmp1}^{proc} + \sum_{\{l,p,m\} \in M^{P-in}} y_{lmp1}^{proc} \qquad \forall \{l,m\} \in M^{L}, t = 1 \tag{20}$$

To ensure that the optimization model does not completely deplete the inventory at the end of the planning horizon (*t*=*T*), a constraint specifying the final minimum inventory quantity must be added.

$$S_{mlT}^{mat} \geq S_{ml}^{End} \qquad \forall \{l,m\} \in M^{L}, t = T \tag{21}$$

Finally, each site has storage capacity constraints.

$$\underline{Q}_{lm}^{stor} \leq S_{lmt}^{mat} \leq \overline{Q}_{lm}^{stor} \qquad \forall \ \{l,m\} \in M^{L}, t \in T \tag{22}$$

Recipe selection

Equations 23 to 28 constrain the selection of recipes. Each process has an offline/idle recipe that can be selected for when the process is not needed. Equation 23 demands that only one recipe (campaign) must be selected during one time period.

$$1 = \sum_{\{l,p,r\}\in R^P} \alpha_{lprt}^{rec} \quad \forall \ \{l,p\} \in P^L, t \in T \tag{23}$$

Equation 24 determines the recipes that are used in the first time period.

$$\alpha_{lpr}^{start} \leq \alpha_{lpr1}^{rec} \quad \forall \ \{l,p,r\} \in R^P, t = 1 \tag{24}$$

Equations 25 to 28 define binary variable β which represents the recipes that are used in at least two consecutive time periods. In the first time period β is equal to zero, as there is no time period before this period. Equations 26 to 28 make the linkage between α and β. Equations 27 and 28 ensure that β is zero, if α is zero in the same or previous time period.

$$\beta_{lprt}^{proc} = 0 \quad \forall \ \{l,p,r\} \in R^P, \ t = 1 \tag{25}$$

$$\alpha_{lprt}^{rec} + \alpha_{lprt-1}^{rec} - 1 \ \leq \ \beta_{lprt}^{proc} \quad \forall \{l,p,r\} \in R^P, \ t \in T \tag{26}$$

$$\beta_{lprt}^{proc} \ \leq \alpha_{lprt-1}^{rec} \quad \forall \{l,p,r\} \in R^P, \ t \in T \tag{27}$$

$$\beta_{lprt}^{proc} \ \leq \alpha_{lprt}^{rec} \quad \forall \{l,p,r\} \in R^P, \ t \in T \tag{28}$$

Production

Processes must be permanently utilized (or idled) during a time period. The available processing hours are equal to the number of hours during a time period minus scheduled maintenance shutdown and lost time during changeovers. As there is no changeover in the first time period, equation 29 only considers shutdown hours.

$$\sum_{\{l,p,r\}\in R^P} h_{lprt}^{rec} = H_{lpt}^{proc} - \varepsilon_{lpt}^{proc} \qquad \forall \ \{l,p\} \in P^L, \ t = 1 \tag{29}$$

$$\sum_{\{l,p,r\}\in R^P} h_{lprt}^{rec} = H_{lpt}^{proc} - \varepsilon_{lpt}^{proc} - \left(1 - \sum_{\{l,p,r\}\in R^P} \beta_{lprt}^{proc}\right) H_{lp}^{changeover} \qquad \forall \ \{l,p\} \in P^L, \ t \in T > 1 \tag{30}$$

Each recipe has minimum and maximum throughput boundaries (tons/hour).

$$h_{lprt}^{rec} \underline{Q}_{lpr}^{proc} \leq y_{lprt}^{rec-tot} \leq h_{lprt}^{rec} \overline{Q}_{lpr}^{proc} \qquad \forall \{l,p,r\} \in R^P, t \in T \tag{31}$$

Production hours are bounded between minimum campaign length and available processing hours including shutdown hours.

$$\alpha_{lprt}^{rec} H_{lpr}^{camp} \leq h_{prt}^{rec} \qquad \forall\, l \in L^{mill}, p \in P_l^{mill}, r \in R_p^{proc}, t \in T \tag{32}$$

$$h_{lprt}^{rec} \leq \alpha_{lprt}^{rec}(H_{lpt}^{proc} - \varepsilon_{lpt}^{proc}) \qquad \forall\, l \in L^{mill}, p \in P_l^{mill}, r \in R_p^{proc}, t \in T \tag{33}$$

Equations 34 to 36 are related to the mass balance. Equation 34 links the material conversion from feedstock to products. Linear recipe functions are used to represent process where raw material consumption depends on the utilization rate of the equipment employed. Equation 35 relates the material output to the total output of a process, while equation 36 aggregates the total output of a material during one time period.

$$x_{lmpt}^{proc} = \sum_{\{l,p,r,m\} \in M^{R-in}} a_{lprm}^{input} y_{lprt}^{rec-tot} \qquad \forall\, \{l,p,m\} \in M^{P-in}, t \in T \tag{34}$$

$$y_{lprmt}^{rec} = a_{lprm}^{output} y_{lprt}^{rec-tot} \qquad \forall\, \{l,p,r\} \in R^P, \{l,p,r,m\} \in M^{R-out}, t \in T \tag{35}$$

$$y_{lmpt}^{proc} = \sum_{\{l,p,r,m\} \in M^{R-out}} y_{lprmt}^{rec} \qquad \forall\, \{l,p,m\} \in M^{P-out}, t \in T \tag{36}$$

Processes require or produce steam and/or electricity for their operation. Equations 37 to 40 calculate the steam and electricity production/consumption of processes based on the recipe used.

$$v_{lpt}^{output} = \sum_{\{l,p,r\} \in R^P} b_{lpr}^{output-steam} y_{lprt}^{rec-tot} \qquad \forall\ \{l,p\} \in P^L, t \in T \tag{37}$$

$$v_{lpt}^{input} = \sum_{\{l,p,r\} \in R^P} b_{lpr}^{input-steam} y_{lprt}^{rec-tot} \qquad \forall\ \{l,p\} \in P^L, t \in T \tag{38}$$

$$w_{lpt}^{output} = \sum_{\{l,p,r\} \in R^P} b_{lpr}^{output-elect} v_{lpt}^{output} \qquad \forall\ \{l,p\} \in P^L, t \in T \tag{39}$$

$$w_{lpt}^{input} = \sum_{\{l,p,r\} \in R^P} b_{lpr}^{input-elect} y_{lprt}^{rec-tot} \qquad \forall\ \{l,p\} \in P^L, t \in T \tag{40}$$

The steam balance must be satisfied. Enough steam must be produced by boilers and other steam producing equipments to satisfy the needs of other steam consuming processes. However, extra steam may be produced and vented off if not necessary, as represented in equation 41.

$$\sum_{\{l,p,r\} \in R^P} (v_{lpt}^{output} - v_{lpt}^{input}) \geq 0 \qquad \forall\ \{l,p\} \in P^L, t \in T \tag{41}$$

5. Case study

An example, including two biorefinery design options, has been considered. A mixture of wood chips, forest residues, sawmill residues, and hog fuel is used as feedstock. The product portfolio involves succinic acid (SA), malic acid (MA) and lactic acid (LA). Xylitol is produced as a coproduct. All three products are produced in similar fermenters, after pre-treatment processing steps. SA and MA can be recovered in a similar recovery system, but LA needs a specific recovery system. Two process alternatives have been considered (Fig. 3). In alternative B-1 (Fig. 3a), there are two separate parallel lines, each including a fermentor, which is flexible, and a recovery system. The first line produces LA and the second line produces SA and MA in different production modes, because one recovery system can be used for both products. In the second alternative (B-2), an SA/MA recovery system is added to the LA production line to increase the level of flexibility. The required changes that should be made to this production line are illustrated in Fig. 3b. In this way, this line can produce LA, SA or MA in different production modes based on the recipe that is used on this line. One of SA/MA and LA recovery systems is always in standby mode. According to market conditions, the proper recipe is utilized and the fermentor produces one of the products and the relevant recovery system is used, while the other recovery system will be out of operation. As mentioned previously, changeover to another recipe causes changeover time and cost.

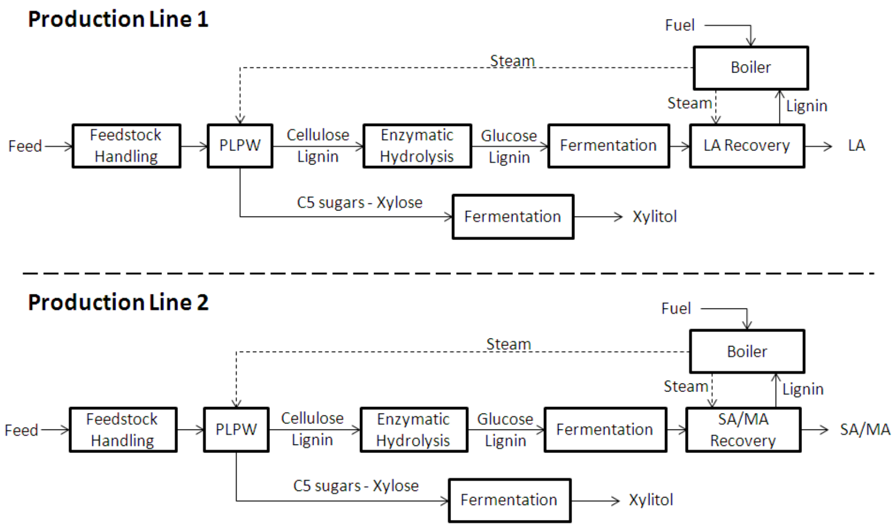

Fig. 3a. Design option B-1

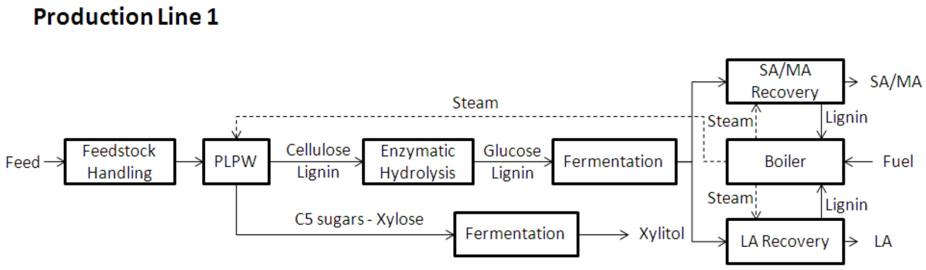

Fig. 3b. First production line in design option B-2

Nine market scenarios have been defined to reflect market volatility into the problem. Scenarios are defined in terms of product price and demand change over one year. Scenarios are depicted in Fig. 4. The graphs only show the spot price and demand. The contractual price is the starting price of each year. First scenario is the base case in which both price and demand follow a sinusoidal trend. Scenarios 2 and 3 represent pessimistic and optimistic cases during which price and demand decrease and increase, respectively. In the next three scenarios (scenarios 4, 5 and 6) the price and demand of one product increase, while those of other two products decrease. In the last three scenarios (scenarios 7, 8 and 9) the price and demand of one product decrease, while those of two other products follow the sinusoidal trend of the base case scenario. Table 1 describes the market scenarios.

Scenario name	Scenario description
Sc.1	Base case: Sinusoidal trend for price and demand for all products
Sc.2	Pessimistic: Price and demand of all products decline
Sc.3	Optimistic: Price and demand of all products grow
Sc.4	MA market grows, SA and LA market crash
Sc.5	SA market grows, MA and LA market crash
Sc.6	LA market grows, SA and MA market crash
Sc.7	MA market crashes, SA and LA markets follow the base case trend
Sc.8	SA market crashes, MA and LA markets follow the base case trend
Sc.9	LA market crashes, SA and MA markets follow the base case trend

Table 1. Scenario description

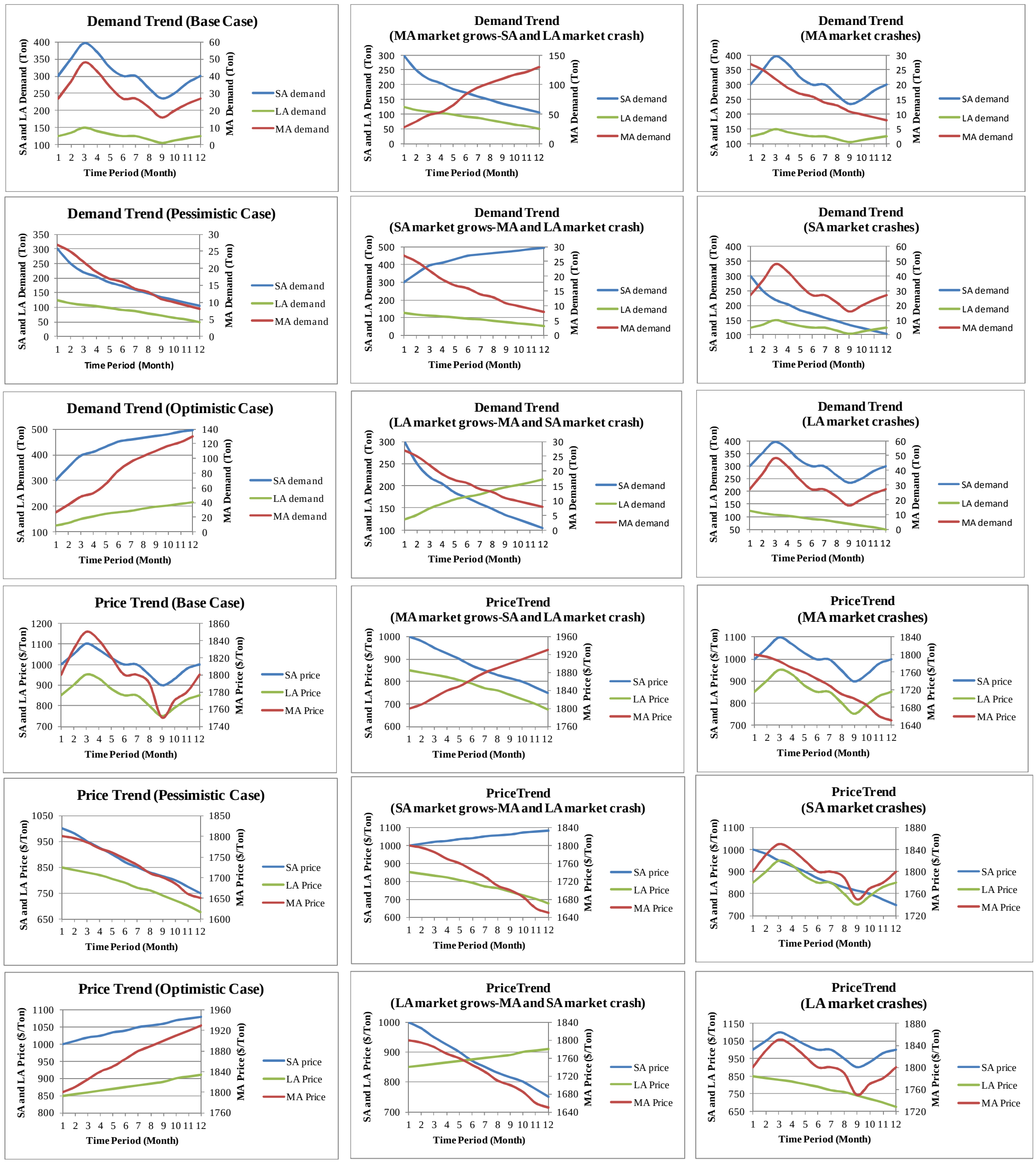

Fig. 4. Market scenarios

6. Applications

As mentioned earlier in this paper, metric of flexibility can be used either for design purposes, or in comparing design options. In this section, the first application is studied under the theme of targeting the level of flexibility, and afterwards, the second application, i.e. comparing different design options, is investigated.

6.1. *Targeting the level of flexibility*

In flexibility design problems, the design is unknown and the problem is to find the optimal design of a system considering the costs incurred by that design. A design representing a higher degree of flexibility will have a lower probability of encountering an infeasible operating condition, but at a higher cost. Two major areas have been considered by Grossmann, Halemane and Swaney (1983): optimal design with a fixed degree of flexibility, and design with an optimal degree of flexibility. In the first type of problem, the degree or level of flexibility is known, either by a discrete set of required operating conditions, or by requiring feasibility of operation when a set of uncertain parameters varies between fixed bounds (Grossmann, Halemane & Swaney, 1983). But in the second type of problem, the desired degree of flexibility is not known, and a design with the optimal degree of flexibility must be identified. The optimal degree of flexibility does not necessarily imply the highest degree of flexibility, because the other criterion, which is the cost of the design, is important in determining optimality of a design. In fact, design with optimal degree of flexibility addresses problems which needs establishing a tradeoff between the cost of the plant and its flexibility. Problems in this category have evolved from flexibility-index problems (Swaney & Grossmann, 1985) to stochastic flexibility-index problems (Pistikopoulos & Grossmann, 1988) and expected stochastic flexibility-index problems (Straub & Grossmann, 1993).

As mentioned, the main approach in flexibility design is doing a trade-off between flexibility and cost of flexibility. This cost implies either the cost of modifications needed for retrofit design or the cost associated with a higher flexibility for a Greenfield design. Therefore, SC costs are typically ignored in such calculations while they constitute a considerable portion of capital and operating cost. A retrofit or a Greenfield design, which, by improving the flexibility, affects the production capability of the system, will have the following effects on the SC:

- In the case of flexible processes that can produce several products in different production modes with different volumes, the production sequence, i.e. recipes that can be used, as well as the production volume is not obvious. A deterministic sequence can be used, but, as will be shown further in this article, a deterministic sequence cannot result in the highest profit. In fact, calculating the profit of a flexible production system without a SC analysis is impossible due to the ambiguity of the production scheme. A SC analysis can determine the optimum production scheme and calculate the associated profit.

- As a result of change in production capacity, the procurement, transportation, and selling costs and strategies will be different. Only a SC analysis can takes into account all these changes.
- The inventory levels and storage capacity will also be different. Again, a SC analysis can calculate the inventory level of each product according to the production scheme and determine the storage capacity required for each product.

In this part of the work, we try to target the level of flexibility using the SC-based analysis. In this way, SC cost and its profitability can be reflected at the design level. The SC model was run for option B-1 in case of all market scenarios. The SC profit was calculated for different levels of flexibility and for each market scenario. Fig. 5 shows the profit of each flexibility level in case of market scenario realizations. As can be observed, profit improves with increasing flexibility up to 30%. Above 30%, the profit is not improved due to market conditions.

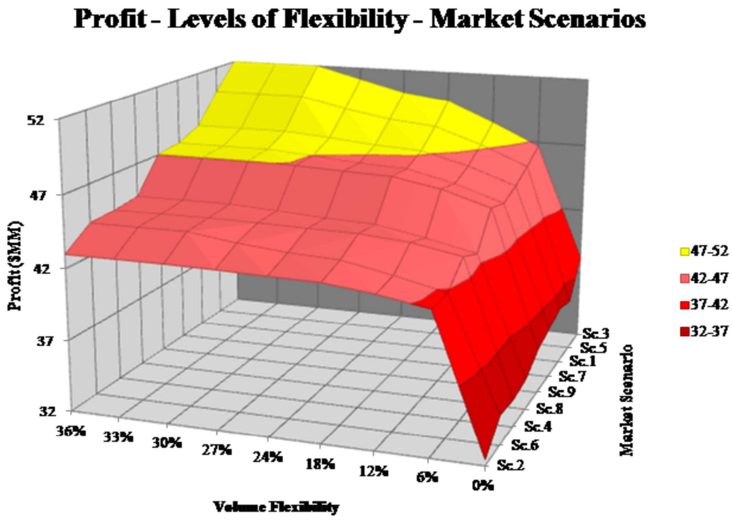

Fig. 5. SC profit of each level of flexibility in case of market scenario realizations

Fig. 6 illustrates the capital cost required for each flexibility level. In calculating the capital cost needed for each flexibility level, the modifications that must be made on the SC have been considered. Such modifications involve slight modification in storage and transportation capacity. As can be seen in Fig. 6, from 0% to 24% volume flexibility, the increase in the capital cost is not significant, because the process has an inherent flexibility and with some slight modifications the level of flexibility is improved. In order to go beyond this level, major modifications are required to be done on the process, which incur more cost. Moreover, with more flexibility, more capacity will be available and the capital cost required for the SC will grow. As a result, the capital cost increases more sharply after 24% volume flexibility.

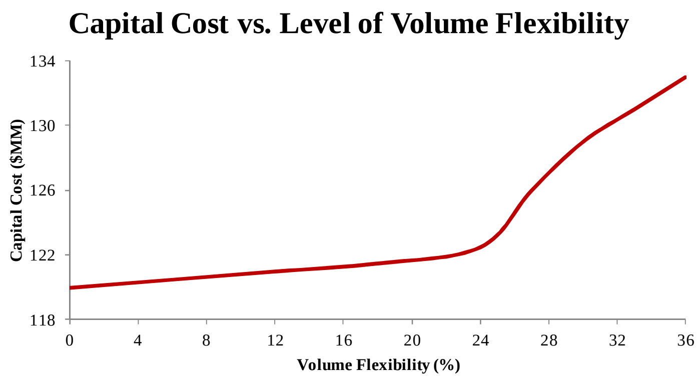

Fig. 6. Capital cost for levels of volume flexibility

To make the final decision, a simple profitability estimation is done using return on investment (ROI), which is defined as profit divided by the capital cost. The result is shown in Fig 7. Up to 24% flexibility, the profitability increases with flexibility. Thus, the increase in capital cost due to flexibility increase can be compensated by the profit improvements. In flexibility levels higher than 24%, the capital cost rise plays the major role and profit improvement in this range is not enough to pay off the extra capital cost. Hence, 24% can be targeted as the optimum level of flexibility. In this way, MF can be used to determine the target level of flexibility for a design option by bringing the SC-level profit up to the process design level.

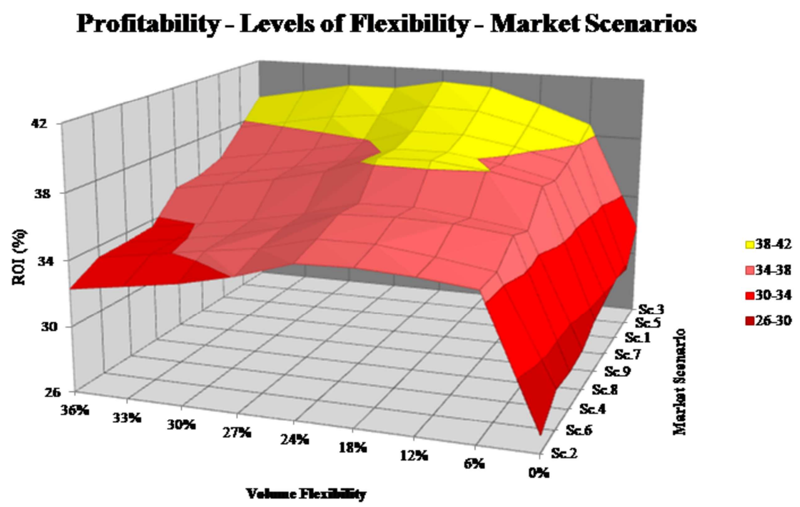

Fig. 7. Profitability of each level of flexibility in case of market scenario realizations

6.2. *Identifying flexible design options*

Another application of MF is in comparing several design options and identifying the most flexible one among others. The same SC analysis is used for this purpose. SC model is run for all design options in case of all market scenario realizations and the SC profit as well as MF is calculated. Product flexibility is acquired by changing the recipes, i.e. changeover, and volume flexibility is done by changing the production rate. The model was run for three cases; design option B-1 with a deterministic recipe sequence and no deviation in volume production (referred to as “No Flexibility”), design option B-1 with enabling the SC model to choose the recipes (referred to as “B-1”), and design option B-2 with enabling the SC model to choose the recipes (referred to as “B-2”). Fig. 8 shows the recipes that are used in the fermentor of the second production line for “No Flexibility” and “B-1” cases for the base case market scenario calculated by the SC framework.

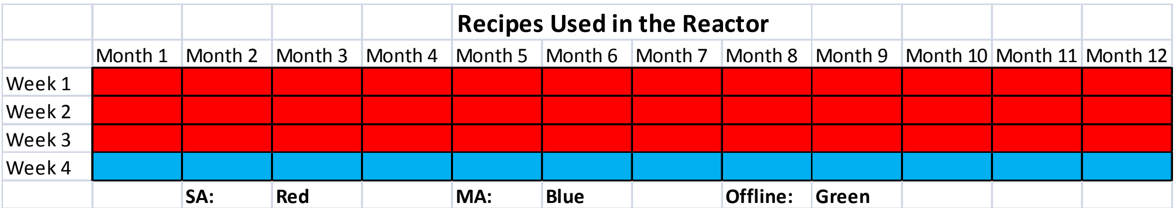

Fig. 8a. Recipes used in second fermentor in “No Flexibility” case; base case market scenario

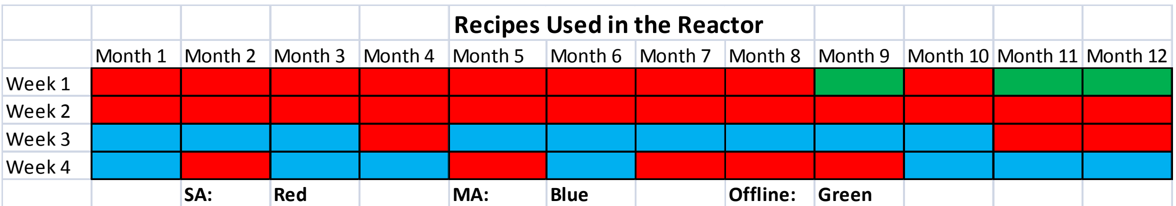

Fig. 8b. Recipes used in second fermentor in “B-1” case; base case market scenario

It is seen that the SC model chooses a different recipe sequence in order to maximize the profit. Fig. 9 depicts the production level of each product in the second fermentor for these two cases for base case market scenario. Production level in “No Flexibility” case is uniform, while in “B-1” case, the production level changes based on market conditions.

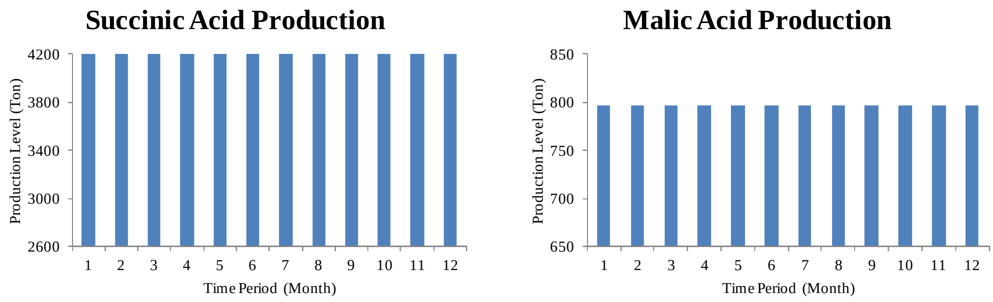

Fig. 9a. Production volume in second fermentor “No Flexibility” case; base case scenario

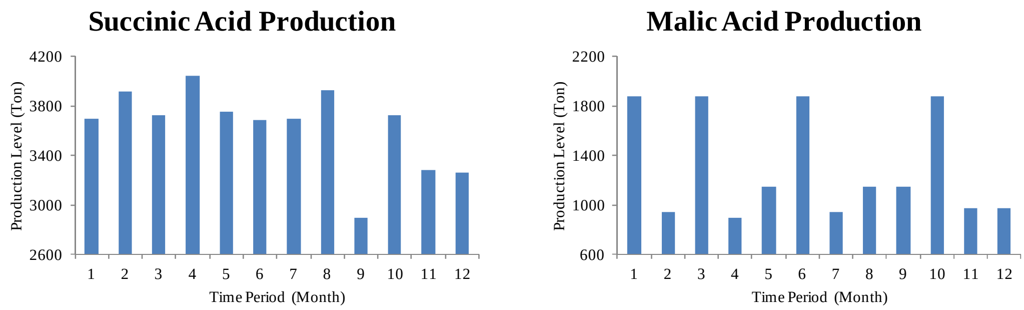

Fig. 9b. Production volume in second fermentor “B-1” case; base case market scenario

Table 2 shows the profit and flexibility calculated by SC model for three cases and all market scenarios. The results are illustrated graphically in Fig.10. It is clear that the profits of flexible cases are higher than that of “No Flexibility” case. The flexibility metric for option B-2, which has more potential for flexibility, is higher for all scenarios. Profit is also higher for this option and that shows more flexibility results in more profit for these specific options. Again, the profitability must be estimated so that the capital cost and its increase for the more flexible option is considered in our analysis. Using average profit, a simple return on investment (ROI) was estimated. Fig. 11 shows how profitability changes with MF. As MF increases, profitability improves. Thus, although extra capital should be spent on more flexible option, this extra capital is well compensated by the increase in flexibility. Increase in MF means that the potential for flexibility is used more in the design option. Therefore, option B-2 can be interpreted as a more flexible design option.

		Sc.1	Sc.2	Sc.3	Sc.4	Sc.5	Sc.6	Sc.7	Sc.8	Sc.9	Avg. Profit	ROI	Avg. MF
No Flexibility	Profit	35.39	30.89	37.22	30.96	35.48	32.65	35.35	32.02	34.42	33.82	27.90%	0
	MF	0%	0%	0%	0%	0%	0%	0%	0%	0%			
B-1	Profit	37.50	33.38	43.78	37.25	40.45	33.97	37.07	34.57	35.53	37.05	30.57%	14%
	MF	13.71%	14.60%	16.29%	13.15%	12.19%	15.30%	13.43%	16.09%	12.90%			
B-2	Profit	45.02	40.46	49.30	43.78	43.20	43.05	44.38	42.54	42.38	43.78	33.33%	17%
	MF	17.63%	18.15%	21.99%	18.06%	20.61%	13.21%	14.50%	13.73%	16.67%			

Table 2. Profit and MF calculated for all cases and market scenarios

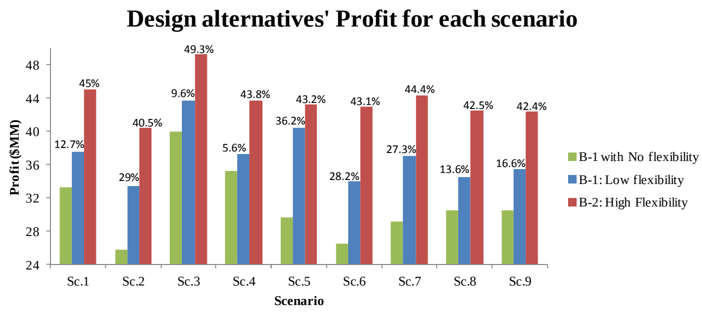

Fig. 10. Profit for three design cases for all market scenarios

As illustrated by Fig. 11, the "No Flexibility" case, which has the least MF (MF=0, meaning that there is no change in production volume), has the worst profitability and the lowest MR. As flexibility increases, the robustness against market volatility improves. For case "B-1" (MF=0.13), the profitability improves by two percent, while the MR increases by 2. Case "B-2" (MF=0.17) has the highest profitability (ROI=33.5%) and the best robustness (SD=\$2.58MM). The result demonstrates that, for these specific design options, flexibility will improve both profitability and robustness. Hence, by investing more in a more flexible design option, the project will have a better return and moreover, it will have a more robust response to market volatility and the deviation of profits from the base case profit is less than that of the less flexible options. As shown by the MF, the higher potential for flexibility in option B-2 is used very well by the SC framework to ameliorate the profitability and robustness.

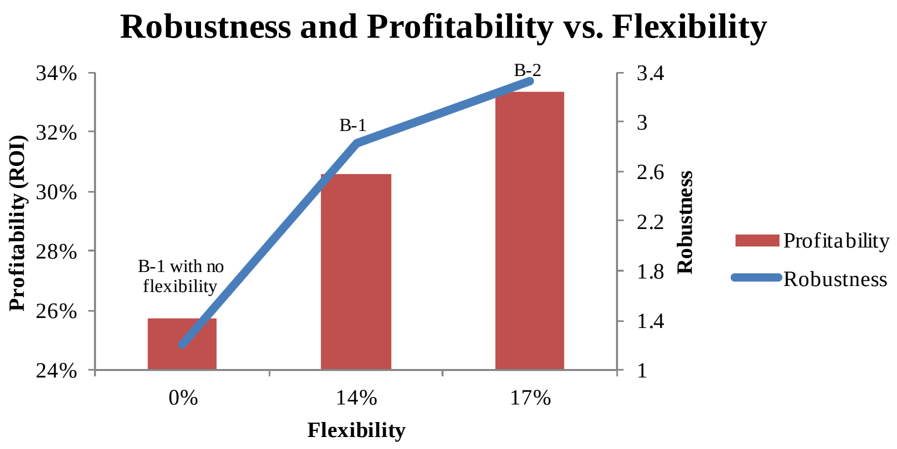

Fig. 11. Robustness and profitability vs. flexibility

6.3. *Conditional value-at-risk (CVAR)*

As discussed by Verderame and Floudas (2011), CVAR aims at guarding against realization of uncertain parameters by going beyond the expected evaluation when expressing the uncertainty of system parameters. A loss function must be defined as a function of decision vector and uncertain parameters with a probability distribution. Using the loss function and the acceptable loss level, two constraints are added to the optimization formulation which restrict the evaluation of the system's variables according to a user-specified risk-aversion parameter.

Inspired by (Verderame & Floudas, 2011), we add a CVAR-like parameter to the SC framework. Contractual order acceptance percentage (OA) is considered to study the risk associated with acceptance/rejection of the contractual orders. A high OA implies less risk, because contractual orders are fixed in price and amount over the long term and thus they can secure the profit. On the other hand, a low OA connotes more spot orders which might improve the profit, as spot prices are sometimes higher than the contractual prices, but poses higher risks, because spot demands are not certain. A constraint is added to the optimization formulation, in which OA should be bigger than a risk factor. Probability of market scenarios are not considered in this study. The added constraint is shown in equation 3:

$$\frac{\textit{Volume associated with the accepted contractual orders}}{\textit{Volume associated with all contractual orders}} > \alpha \qquad (3)$$

where α is the risk parameter. Probability of market scenarios has not been considered in this study. For this part of the study, market scenarios are modified slightly. Market scenarios represent only price volatility, and demand changes follow the base case demand trend. In this way, a specific OA value means one order acceptance pattern for all market scenarios, while, if the demand trend changes in each scenario, an OA value will be associated with a different order acceptance pattern for each scenario, and hence, the results of different scenarios cannot be compared. A worst case scenario is also added to the market scenarios. In this scenario, the spot market is very weak. This scenario is generated to show the risk of rejecting contracts when spot market is weak.

Table 3 shows the result of CVAR study for design option B-1. SC model was run for market scenario 1, 2, 3, 4, 5, 7, 8 and worst case. The profit was calculated for several levels of OA. The maximum profit happens in different percentages (highlighted in bold), showing that there is not one optimum percentage for all scenarios. In 80% OA, the average profit and the robustness metric has the highest value, except compared to the 100% OA which has a low profit, but the best robustness. Therefore, 80% OA can be chosen over lower OAs, and then be compared to 100% OA. Decision makers with low risk tolerance may choose 100% OA which has better robustness, while those with higher risk tolerance can choose 80% OA which has the highest profit. The results are shown in Fig. 12 and Fig. 13 graphically.

OA%	Sc.1	Sc.2	Sc.3	Sc.4	Sc.5	Sc.7	Sc.8	Worst	MR	Profit
22.03%	37.57	34.16	40.32	34.33	38.27	37.47	34.25	7.66	0.93	33.01
28.81%	39.52	36.11	42.27	36.28	40.22	39.43	36.21	9.28	0.98	34.92
49.15%	45.08	42.08	**47.77**	42.25	45.86	44.98	42.17	16.33	1.19	40.82
50.85%	45.16	42.29	47.77	42.46	**45.92**	45.06	42.38	16.87	1.22	40.99
72.88%	**45.19**	44.36	45.97	44.53	44.43	**45.09**	44.46	24.16	1.93	42.28
79.66%	45.17	**44.80**	45.52	**44.97**	44.28	45.07	**44.90**	25.95	**2.24**	**42.59**
100.00%	35.94	35.35	38.33	35.35	36.12	35.94	35.35	**34.00**	**9.74**	**35.80**

Table 3. Profit, robustness and average profit for option B-1 in case of different OAs and market scenarios

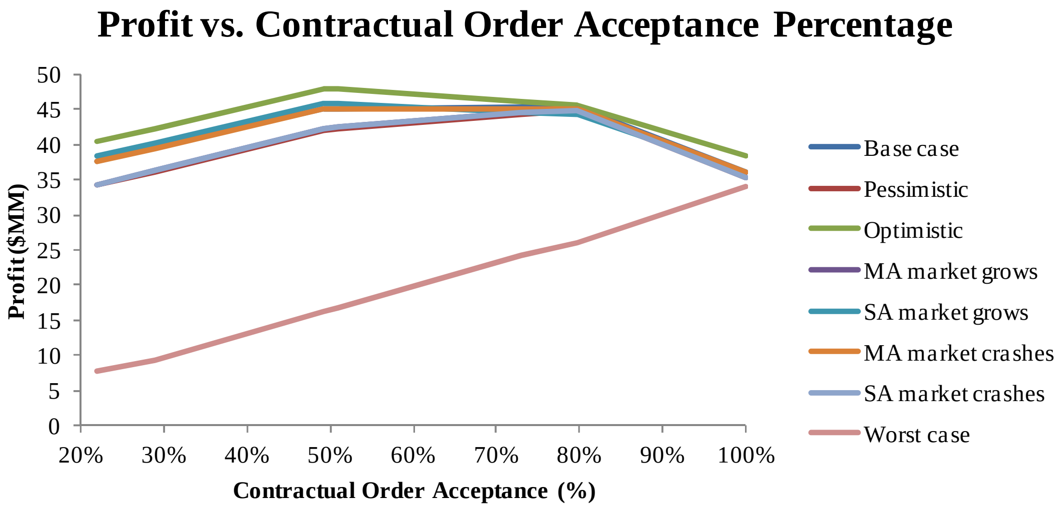

Fig. 12. Profit vs. OA

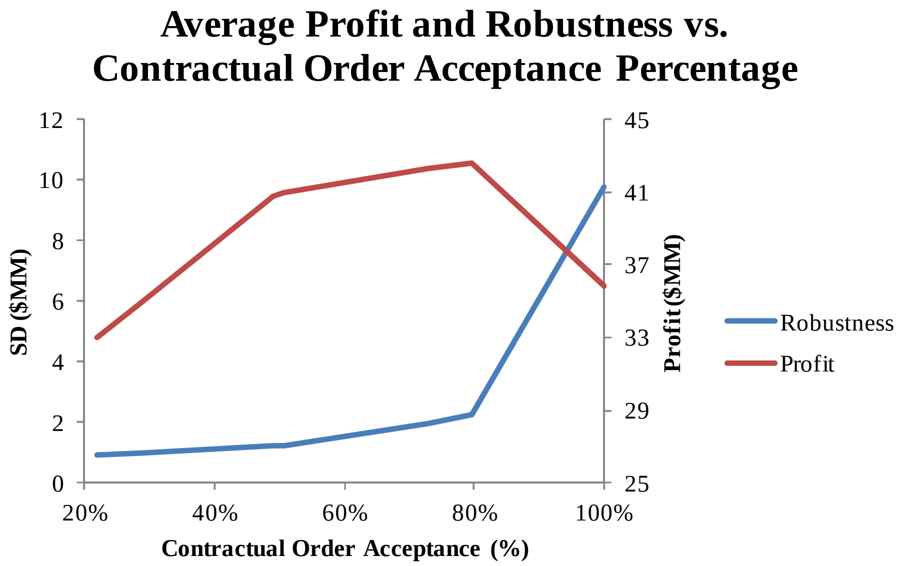

Fig. 13. Average profit and robustness vs. OA

Fig. 14 demonstrates the percentage of the accepted orders resulted in the highest profit for each scenario. For the optimistic scenarios (3 and 5), the maximum profit happens in lower OAs compared to other scenarios, because in these scenarios the spot market is strong and more spot orders are fulfilled and lower OA results in higher profit. By contrast, for pessimistic scenario (2) and scenarios with declining trends (4, 7 and 8), more contracts are accepted and fulfilled, because the spot market is weak. For the worst case scenario, the maximum profit is acquired at

100% OA, because the spot market is not profitable at all and at 100% OA, where all contracts are made, the profit is maximized. Fig. 15 reveals how production capacity is dedicated to spot and contractual orders for the OAs resulted in the highest profit. Again, for the optimistic scenarios more capacity is dedicated to spot orders. On the contrary, for other scenarios the capacity dedicated to contractual orders is bigger.

Fig. 14. OA for spot and contractual orders

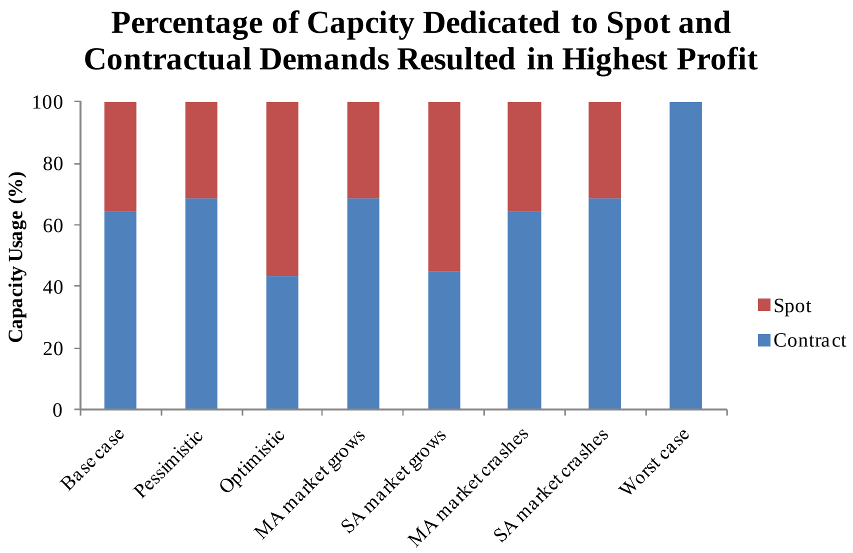

Fig 15. Capacity utilization for spot and contractual orders

7. General and concluding remarks

To mitigate the risks of market volatility, the processes and the SC must be designed flexible to have a robust response to changing market. Although more flexible design alternatives are more capital intensive, the results show that this capital will be very well paid off by increasing the capability of the system to react properly to market changes and a more flexible alternative will be more profitable and robust. Metric of flexibility (MF) and metric of robustness (MR) can give a good insight on how a SC reacts against market volatility. Such metrics can quantify the performance of several SCs in different market conditions. Moreover, in an MCDM several metrics are required in order to reflect the performance of design options/strategies into the decision making process. Such metrics can be used along with economic, environmental and social metrics in an MCDM and enable the decision makers to choose a viable option.

The CVAR studies show that optimum contractual percentage of order acceptance (OA) is different for each market scenario. This study demonstrates that lower risks may imply lower profit and thus, an appropriate trade-off analysis ought to be performed to choose the right OA.

This work presented for the case of added value chemicals. It should be investigated whether profitability and robustness will increase with flexibility in case of commodities or not. In future works, the introduced metrics will be applied for continuous process options producing commodity chemicals.

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APPENDIX C - Article: Incorporating flexibility design into supply chain for the forest biorefinery

INCORPORATING FLEXIBILITY DESIGN INTO SUPPLY CHAIN DESIGN FOR FOREST BIOREFINERY

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ABSTRACT

For a forestry company to improve its business model, it should, on one hand, diversify its revenue, and on the other hand, change its current manufacturing culture, which focuses on capacity management and neglects supply chain (SC) profitability. This culture will be changed by applying novel SC operating policies which help to maximize SC profit by exploiting production flexibility. The level of flexibility should lead to maximum SC profit and must have an acceptable return on investment. Desired level of flexibility must be targeted at the design stage. As the ultimate goal is to maximize the SC profit, SC profitability must play a key role in targeting the level of flexibility. The goal of this paper is to show how an SC-based analysis can be used for targeting the level of flexibility in biorefinery processes. For a finite number of design alternatives with different potentials for flexibility, the SC-based analysis targets the operating window of each design alternative, and evaluates their performance under different market conditions based on the impacts of the design of each alternative on operational activities.

Key words: Forest Biorefinery, Pulp and Paper, Flexibility, Supply Chain Design

INTRODUCTION

For a forestry company to improve its business model in the current market situation, it not only should diversify its revenue, but also must change its current manufacturing culture, which focuses on capacity management and neglects the profitability of the entire SC. According to the phased strategy for the forest biorefinery (FBR) implementation [1] shown in Fig. 1, revenue diversification will be achieved by means of “technology disruption” by producing building-block chemicals, and ideally, in the longer term, by increasing revenues by producing added-value derivatives. On the other side, manufacturing culture will be changed via “business

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disruption," through applying novel SC operating policies and exploiting production flexibility, in the short term, and by using advanced ERP and decision-making tools in the long term.

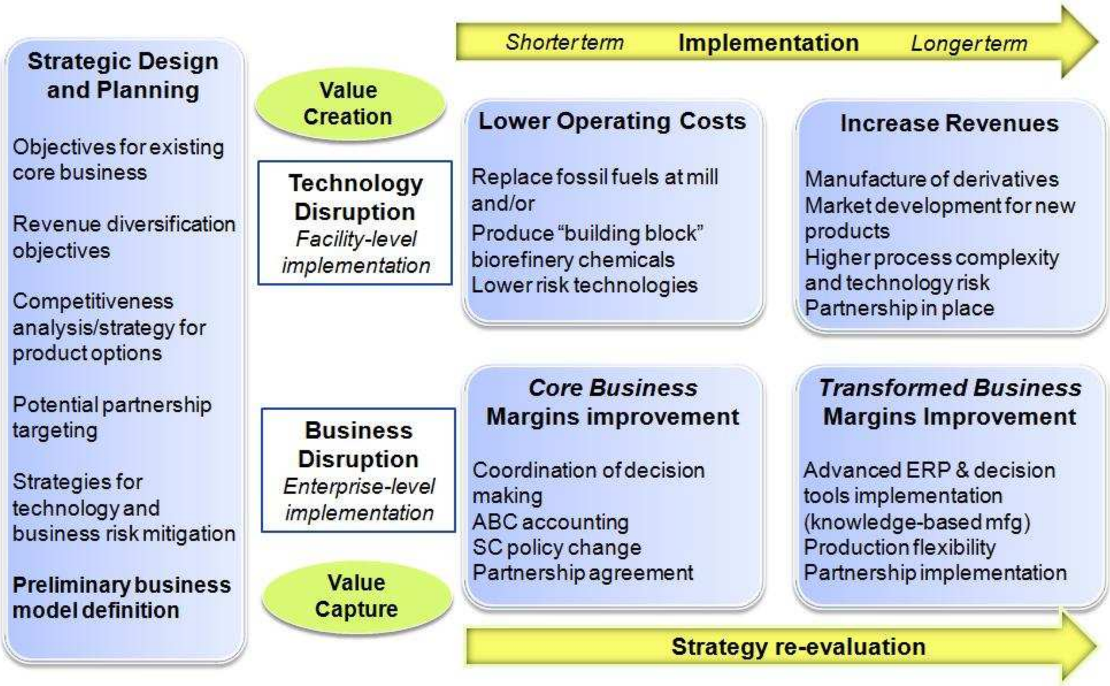

Fig 1 - Strategic implementation of the biorefinery.

SC analysis can play a key role for a successful "business disruption". In the short term, to mitigate the risks of market volatility, companies should focus on improving their margins by implementing a margins-based SC operating policy and better exploiting the process flexibility [1]. SC optimization can be used to carry out product planning over different time horizons and to identify tradeoffs between product orders and anticipated supply and demand. Moreover, over the long term, companies should base their strategic decisions on a bottom-up approach, i.e. designing/redesigning the SC based on the impact of the design on operational activities. The margins-based and the bottom-up approaches imply profound changes in the way forestry companies do business today, which is equivalent to business disruption.

SC analysis is widely used in different industries. A review of advances in SC problems and modelling is provided by Shah [2] and Papageorgiou [3]. More specifically, application of SC-based analysis in biorefinery design is getting attention. Sammons et al. (2008) proposed a general systematic framework including SC optimization for optimizing product portfolio and process configuration in integrated biorefineries [4]. Tursun et al. (2008) developed a mathematical programming model that determines optimal locations and capacities of biorefineries, delivery of bioenergy crops to biorefineries, and processing and distribution of ethanol and co-products across Illinois [5]. Slade et al. (2009) analyzed the role of SC design on determining the viability of commercial cellulosic ethanol projects in Europe [6]. Eksioglu et al. (2009) developed a mathematical model to analyze and manage a biomass-to-biorefinery SC [7]. Mansoornejad et al. (2010) introduced a hierarchical methodology to integrate product portfolio design with SC network design in the FBR [8].

In this paper we try to show how an SC-based analysis can reflect SC design into process design and can be used for targeting the level of flexibility in FBR processes. The rest of the paper is organized as follows. First, some key concepts used in the paper are briefly reviewed. Next, the problem statement is given. Then, the SC optimization model is discussed. Afterwards, the proposed methodology for SC-based analysis is presented. Finally, a case study is presented to concretize the methodology.

Margins-Based Operating Policy

The operating policy in the P&P industry is said to be “manufacturing-centric.” In this industrial sector, the management focus is on capacity planning, and industry participants try to achieve the efficient use of machine capacity [9]. As a result, process efficiency is viewed as the key measure for profitability, and therefore it is believed that minimizing production cost will result in the highest profitability [10]. Moreover, production planning assumes a known set of orders and a fixed sequence of product grades. By treating the manufacturing process as the focal point, inventory and changeover costs are typically ignored or considered separately [9] and SC costs are often neglected [10].

On the other hand, a margins-based policy tries to maximize margins over the entire SC and to produce and select products and orders that ensure the best returns, leaving aside traditional recipes and practices [10]. For an FBR to be successful, the operating policy must shift from a manufacturing-centric approach to a margins-based one, so that the company focuses on maximizing the profit instead of reducing costs. The importance of profit and revenue management compared to cost reduction has been acknowledged by many industries [11].

Bottom-Up Approach

The ultimate goal of margins-based policy is to maximize profit across the entire SC. Therefore, an SC-based analysis tool is needed to show how the flexibility should be managed and exploited at the operational level to maximize SC profit. Moreover, at the process design level, flexibility must be designed in a way that ensures the best performance at the operational level and the attainment of the ultimate goal, i.e., maximizing the SC profit. Hence, SC profitability must be reflected at the process design stage. On the other hand, from a SC design perspective, the SC network should be designed in such a way that the maximum exploitation of flexibility can be obtained. Therefore, an SC-based analysis tool is required to address both aspects: operational and design.

Figure 2 provides a schematic illustration of the linkage between SC analysis, and design and operational decisions.

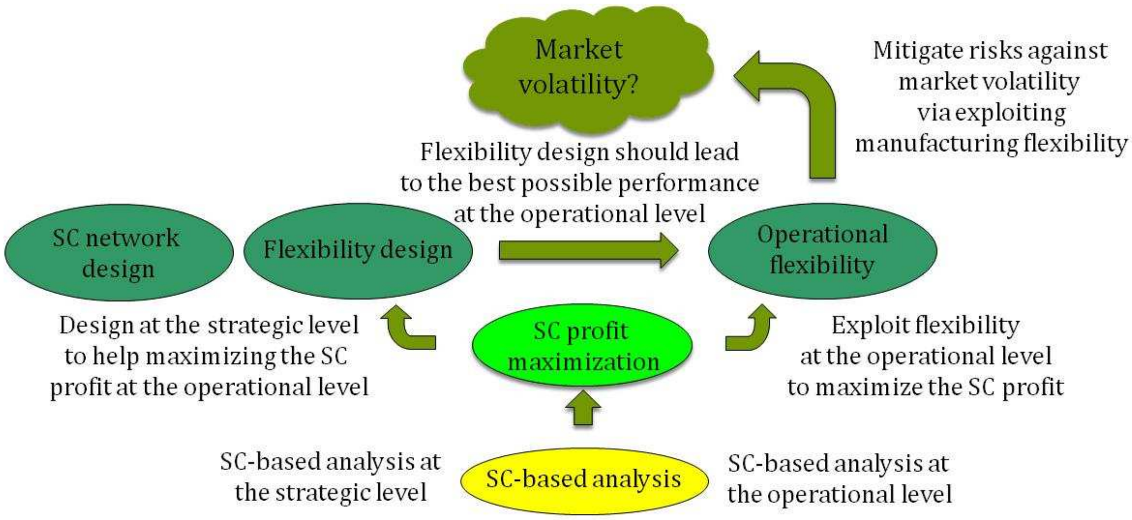

Fig 2 - Linkage between SC-based analysis and design/operational decisions.

Manufacturing Flexibility

Today's chemical market is subject to huge volatilities in terms of price and demand. The price of products changes periodically. The demand is not always certain, and sometimes, despite strong demand, the price is too low for the production of a product to be profitable [12]. On the feedstock side, uncertainty exists in terms of price and availability [7]. To mitigate risks, it is of crucial importance to enhance adaptiveness and reactivity on one hand and to act proactively on the other hand [12]. These capabilities are generally called flexibility. An FBR would be exposed to this kind of volatile environment. Hence, flexibility, of any possible type, must be exploited in an FBR to mitigate risks.

In the chemical engineering context, Grossmann et al. (1983) defined flexibility as the ability of a manufacturing system to satisfy specifications and constraints despite variations that may occur in parameter values during operation [13]. Four major types of flexibility have been widely studied in chemical engineering literature: recipe [14, 15, and 16], product and volume [17, 18, 19, and 20] and process [21, 22, and 23]. The definition of each flexibility type is given in Table 1.

Flexibility	Definition
Recipe [16]	The ability to have a set of adaptable recipes that can control the process output
Product [24]	The ability to change over to produce a new (set of) product(s) economically
Volume [24]	The ability to operate a system profitably at different production volumes
Process [25]	Capability of the process to operate feasibly under changing operating conditions

Table 1 - Types of flexibility and their definition.

Some definitions have overlapping scopes which, for instance, can be seen in the definitions of volume and process flexibility. “Changing operating conditions” in process flexibility definition are mainly temperature, pressure and flowrate. Thus, changing flowrate implies both volume and process flexibility.

The concept of manufacturing flexibility in the FBR implies the ability to produce several bioproducts at different volumes and in different time periods based on product price and demand. This definition is an aggregation of product flexibility and volume flexibility. Manufacturing flexibility implies a justifiable increase in capital and operating cost that is adequately compensated by the ability of the process to manufacture in a flexible manner so that the expected volatility in market conditions can be mitigated.

Problem Statement

In the strategic design of an SC, long-term decisions should be made. Such decisions include type of products, technologies, the number, location and capacity of each type of facility, e.g., plants and warehouses, and the target markets.

The decision as to what biorefinery strategy to take depends on many factors, most of which cannot be reflected in an optimization problem, e.g., understanding the market and market strategies, emerging products and technologies, the capabilities of existing SC assets, and potential partners. In a practical problem, it is difficult to address all these decision variables within a single SC optimization model. Instead, it is preferable to pursue a systematic hierarchical methodology that addresses all these factors in a stepwise manner. Because of the combinatorial aspect of such design problems, the hierarchical methodology might miss the global optimum. However, the methodology presented in this article does not seek to identify a global optimum. Rather, it seeks a set of feasible and practical biorefinery options that a company can strategically implement. Many of the key aspects can be addressed in different scenarios/alternatives instead of being modeled into an optimization formulation. In this way, a simpler model will be solved, with more practical results.

The ultimate goal of this work is to provide a hierarchical methodology that targets the level of flexibility of several design alternatives using an SC-based analysis, which helps considering the SC design issues in flexibility design. The SC-based analysis targets the operating window of several biorefinery options with different potentials for flexibility and evaluates their performance under different market conditions based on the impacts of the design of each option on operational activities. These biorefinery options will be identified by the company's experts based on their experience and knowledge of the company, future forecasts, the assets of the company's existing SC, the potentials of the company for biorefinery implementation, and the potential for forming partnerships with other companies.

SC Optimization Model

The SC model aims to maximize profit across the SC by identifying the tradeoffs between demand and production capabilities and by finding the optimal alignment of manufacturing capacity and market demand. The model exploits the potential for flexibility and determines which orders must be fulfilled, and therefore how much of which products must be produced, how they should be stored, and how they should be delivered to the market to maximize SC profit.

The model used in this paper was inspired by the tactical model introduced in [26]. The objective of the SC model is profit maximization. This model considers the management of a multi-product, multi-echelon SC, including production and warehousing facilities as well as a number of customer zones. Different types of biomass are provided by several suppliers. Production facilities can make one or several products. Processes are either dedicated, i.e. they produce only one product, or flexible, i.e. they are able to produce several products through different modes. Changing from one mode to another incurs changeover cost and time. Processes can be idled or shutdown for scheduled maintenance. The steam required for each process is provided by both fuel and biomass. Warehouses can receive material, either feedstock or product, from different sources and plants, and supply different markets. Each market places demand in two ways: by contract, i.e., for the long term, and on the spot, i.e., for the short term. In case of a contract, specific quantities of products must be sold to the customer in specific time periods. The spot demand can be partially fulfilled. Transportation routes link suppliers, facilities and customers together. The model is formulated as a mixed integer linear programming (MILP) problem with a discrete time horizon of 52 weeks, i.e. a year.

Overall methodology

To achieve a stepwise methodology, some of the abovementioned decisions must be made by other methodologies separately. The set of products is identified by a product portfolio definition/selection methodology. The processes and technologies are chosen through a technoeconomic study. The aspects that will be determined by the hierarchical methodology include:

(1) Flexibility design including the determination of the production capacity as well as the range of production rates for each process, i.e. operating window.

(2) SC network design, including determination of the location and capacity of facilities of each type, as well as partner selection.

The methodology is illustrated in Fig. 3. First, process design alternatives representing different potentials of flexibility are defined. In the second step, SC network alternatives are defined based on the assets of the existing SC and resources that are needed for new products. Then the process and the SC network alternatives are combined to create a set of process-SC network alternatives, called combined alternatives. Then, the SC model is run for different levels of volume flexibility of each combined alternative, in case of several market scenarios. The SC profit of each combined alternative is calculated and using profit and capital costs, profitability of each alternative can be estimated. Moreover, the flexibility and robustness of each alternative against all market scenarios can be determined using relevant metrics, which will be presented further in this paper. These metrics, i.e. profitability, robustness and flexibility, can be used to evaluate the performance of alternatives. In the next sections, the methodology is explained in detail. The methodology has three major steps; process design, SC design, and decision making.

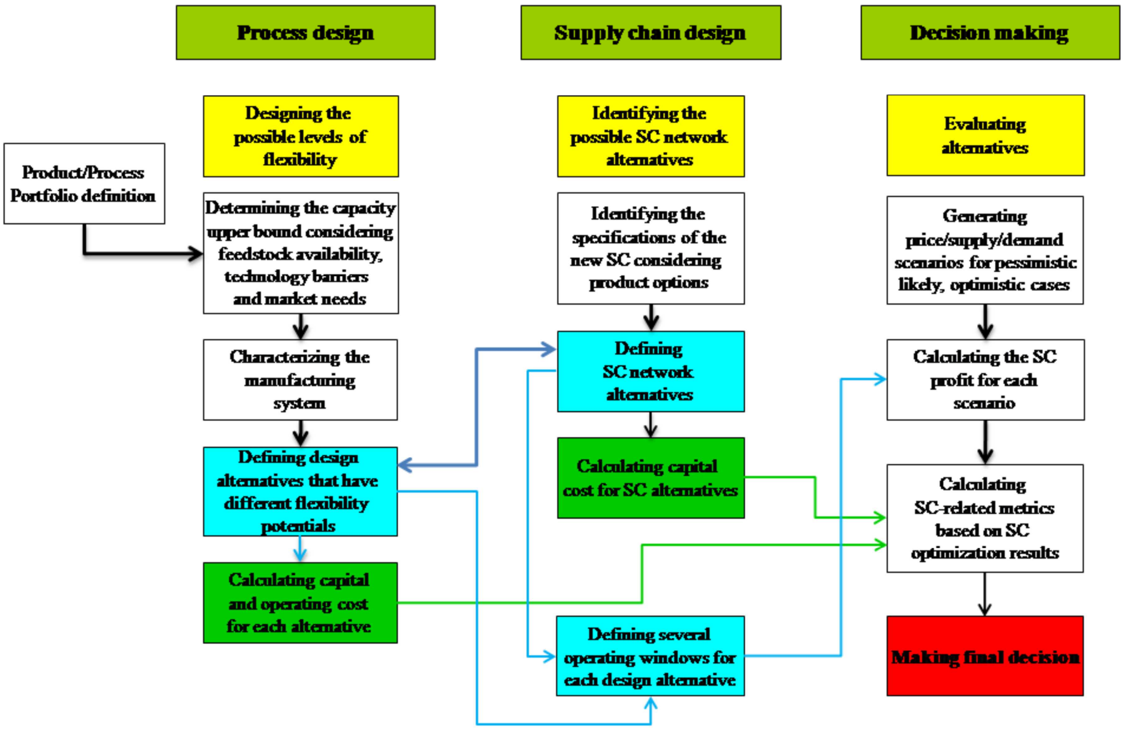

Fig. 3 - Hierarchical methodology for SC strategic design

Process Design

In the first part of the methodology, i.e., process design, there are four steps: determining the upper bound for production capacity, characterizing the manufacturing system in terms of product and volume flexibility to identify the modifications needed for the processes to become more flexible, generating design alternatives with different flexibility potentials, and calculating capital and operating cost for each design alternative.

Determining the Capacity Upper Bound

The maximum possible capacities for each process are identified by considering three major factors: market demand, feedstock availability, and technical barriers. In the case of a biorefinery implementation, feedstock availability is the most important factor in calculating the capacity upper bound. The availability of feedstock from different sources in and around the mill region is studied, and the cost of bringing the feedstock to the mill is estimated. Various factors should be considered in calculating the amount of available feedstock, e.g., price, proximity, seasonality, and transportation. A market analysis is carried out to determine the market size and market share of the targeted products based on the available amount of feedstock. Finally, considering the available technologies and the possible production rates from a technical point of view as provided by the technology providers, maximum capacity is identified.

Characterizing the Manufacturing System

To design a flexible production system, this system must be characterized based on the following aspects:

- Process configuration: It should be verified whether the products can be produced in series, i.e., they are in one product family (Fig. 4.a), or whether they should be produced in parallel lines, because they are not from one family (Fig. 4.b).
- Product flexibility: It should be verified whether the system is a dedicated one in terms of products (Figs. 4.a and 4.b), or whether several products can be produced in a single line in different production modes (Fig. 5).
- Volume flexibility: It should be verified whether the process can handle a range of production rates and whether the inherent flexibility of the process is enough or not.

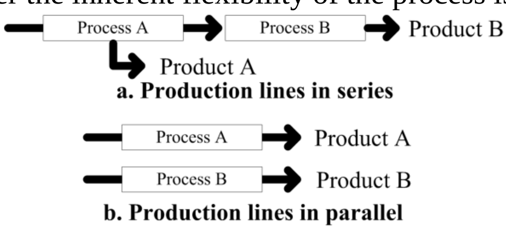

Fig. 4 - Separate production lines: a) in series, b) in parallel.

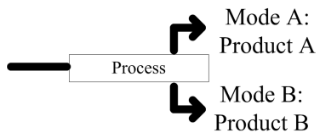

Fig. 5 - Flexible production line.

Defining Design Alternatives with Different Flexibility potentials

The goal of this step is to define several process alternatives, each representing a potential of flexibility. This task is very much case-dependent. Based on the characterization of the manufacturing system, different strategies can be used to increase the flexibility.

Chemical processes are designed to operate at maximum capacity, which is generally called nominal production rate. Under changing conditions the operating rate must change to some extent. The distance (as a percentage of nominal rate) between the lowest point below the nominal production rate, at which the process can operate, and the designed nominal production rate is called the turndown ratio. All chemical processes have an inherent turndown ratio. But sometimes it is desirable to have a greater turndown ratio than the inherent one. A simple way is to divide the production line, or the part of it that limits the process, into smaller lines, so that if the production rate must be decreased, some of these smaller lines can be shut down.

A similar strategy that can be used to make a system more flexible is to add extra equipment or process sections and keep them standby. This strategy will work for increasing capacity. The number of equipment that restricts the process can be increased so that when production increases, more capacity can be provided by the standby equipment.

Calculating Capital and Operating Costs for Each Design Alternative

Finally, the required capital investment for each design alternative and the operating cost associated with the nominal production rates are calculated. These costs will be used to estimate the profitability of each design alternative under different market scenarios. It is assumed that the cost-per-unit of production is fixed. In future works, the SC model will be modified to be able to account for change in production unit costs.

Up to this step, a few number of design alternatives with different potentials of flexibility have been defined. But the flexibility of each process has not targeted yet. As the goal is to incorporate SC design into flexibility design, in the next step the SC network alternatives must be defined and combined with design alternatives. Then, the SC model can be used to target the flexibility of each process.

SC design

In the strategic design of the SC network, decisions are made to redesign an already established SC network with all its existing assets. The SC of a forestry company should be redesigned so that it can be used in the FBR. In this methodology, the SC network design is performed in two steps. First, the specifications of the new SC are identified based on the characteristics of the new product options. Then SC network alternatives are defined. These SC network alternatives will be combined with the process design alternatives defined in the previous part of the methodology, and in the final part, SC optimization is used to calculate the SC profitability of each alternative. Interaction between this part and the previous part is necessary.

Identifying the Specifications of the New SC with Product Options

The SC networks of forest-products companies are in place with their own existing assets. However, some facilities and processing steps are common among all processes in the mill, and therefore similar facilities and assets can be used or redesigned to be able to handle larger volumes.

Biomass receiving, processing, and storage areas in the mills are used regardless of the fate of the biomass, i.e., the final product. Therefore, the design process should identify whether the new processes need the same facilities and whether the existing facilities have enough capacity for the larger amount of biomass that will be brought to the mill. If new or additional facilities are required, it must be investigated how those facilities should be modified or be added to the site to enable the mill to accept more biomass.

On the product side, the characteristics of new products must be taken into account. Each product has specific properties and characteristics which imply specific facilities for storage and transportation. Some products can be stored in warehouses, while others must be stored in tanks. Moreover, some products are transferred by truck or train, while others should be transported in a tanker or by pipeline. Therefore, the specifications of each product must be addressed when defining SC network alternatives.

Defining SC Network Alternatives

Based on the identified specifications, several SC network alternatives can be defined, which reflect the needs of the new SC network as well as the concerns of company experts. Collaborating with other companies whose expertise brings value to the company's capabilities must be considered. Partners can cooperate in producing a product, delivering the product, buying and/or selling the product. An SC network alternative can include new pre-processing steps, new warehouses, new transportation means, and partners.

Calculating capital cost for SC Alternatives

In this step, the capital investment required for redesigning the SC network is calculated. The cost associated with any modification to pre-processing steps, warehousing and transportation system must be addressed.

Targeting flexibility

The goal of this part is to target the flexibility of each design alternative based on its performance in different market conditions. This part contains three steps: after defining several volume flexibility levels for each design alternative, first, a finite number of market scenarios are generated. Then, for all flexibility levels, the SC profit is calculated for each scenario. Then the profitability of each alternative is estimated for each scenario, and the robustness and flexibility of each alternative are quantified.

Generating market Scenarios

To reflect market volatility in decision making, a scenario-based approach is used. Each scenario represents a specific market condition with respect to price, supply, and demand. Scenarios are generated in terms of feedstock availability and product demand, as well as feedstock and product prices. Scenarios are generated to capture pessimistic, likely, and optimistic cases. For strategic decisions, scenarios should be generated for the long term. The values associated with supply, demand, and price can vary over time. Contractual prices and demands imply fixed values during planning period, while spot prices are generally subject to changes. It must be mentioned that addressing internal uncertainties such as model and process uncertainties are out of the scope of this work.

Calculating the SC Profit for Each Scenario/Alternative

In this step, the SC profit of each combined alternative is calculated for all market scenarios using the SC optimization model. The overall problem at this stage can be stated as follows. Given:

- Number and length of time intervals
- Demand and price data for each feedstock, product, market, and time interval for each scenario
- Process configuration based on what was defined in process design section
- SC network configuration based on what was defined in the SC design section
- Capacity data of the nodes of the SC
- Cost parameters, i.e., unit production, transport, and inventory costs;

Find

- Orders to accept: which contracts to make, which spot demand to fulfill
- Production rates of each product for all time intervals
- Flows of materials between the plants, warehouses, and markets
- SC profit

Figure 6 shows this step graphically.

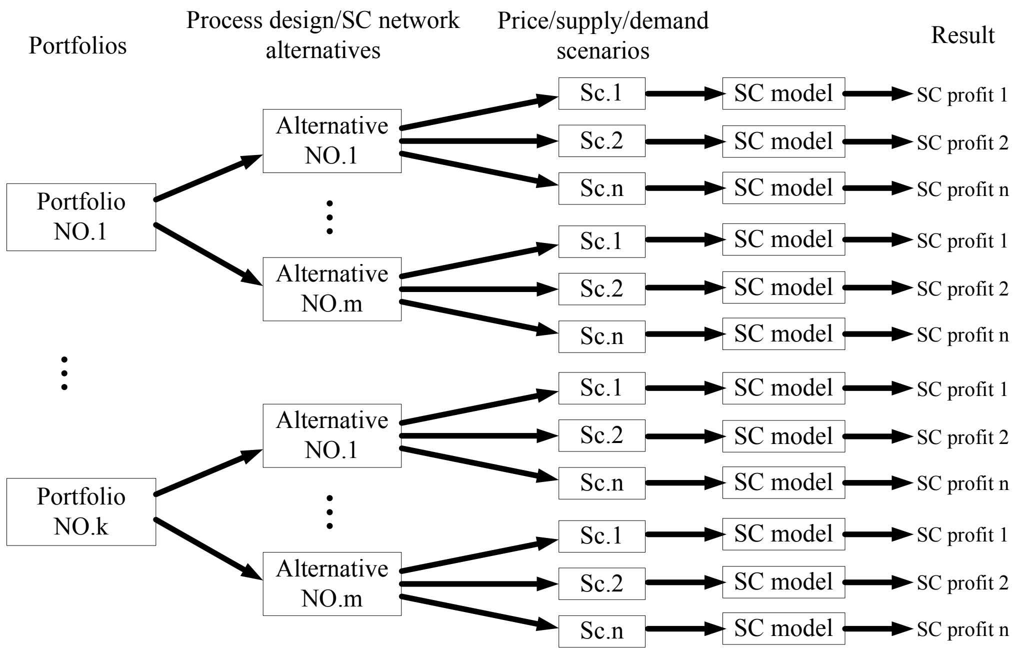

Fig. 6 - SC model inputs and outputs.

Calculating SC-related metrics based on SC optimization results

To evaluate each process/SC alternative, the value of several metrics should be estimated for each alternative. In this paper, SC profitability, flexibility and robustness are used.

There are several profitability estimation methods that can be used to estimate the profitability of a project. In this methodology, return on investment (ROI) is used as the measure of profitability. ROI is a simple measure which is generally used for preliminary design calculations. It does not consider the time value of money, variable depreciation allowance, increasing maintenance costs over the project life, or changing sales volumes [27]. However, because the proposed methodology involves a preliminary design study, ROI can be used as the profitability measure. ROI is defined as the ratio of profit to investment. The most common measures are annual net profit and total capital investment. The net profit is calculated by SC optimization model.

To quantify volume flexibility, equation (1), inspired from work of Voudouris (1996) on qualitative measure of flexibility [28], has been developed:

$$\mathrm{MF} = \sum_{t}\sum_{p}\sum_{m}\left|\frac{C_{mpt}-C_{mp}^{N}}{C_{mp}^{N}}\right| \quad (1)$$

where Cmpt is the amount of product m that is produced on process p in time period t and CNmp is the amount of product m produced on process p by the nominal production rate over the same number of processing hours. This formulation shows the deviation from the nominal production rate and implies volume flexibility.

Klibi et al. (2010) define robustness as the extent to which the SC network is able to carry its functions for a variety of plausible future scenarios [29]. Several robustness metrics have been introduced thus far [30]. Well-known metrics are standard deviation and mean absolute deviation. We use standard deviation as robustness metric, as shown in Eq. (2).

$$\mathrm{MR} = \sqrt{\sum_{Sc}\frac{(\mathrm{Pr}_B-\mathrm{Pr}_{Sc})^2}{N_{Sc}-1}} \qquad (2)$$

where MR is the metric of robustness, Pr_B is the base case profit, Pr_{Sc} is the profit for scenario Sc and N_{Sc} is the number of scenarios. To quantify the downside risk of volatility, profits that are less than the base case profit are considered in this equation.

Making the final decision

At this stage, the final decision can be made using the calculated metrics. In order to account for metrics provided by other analysis tools, an MCDM framework can be used to analyze the performance of each defined option from several perspectives. Figure 7 shows the metrics provided by different analysis tools to be used in the MCDM. MCDM panel weights each metric based on its importance and the framework will identify the best option. The detail of the MCDM is not in the scope of this work.

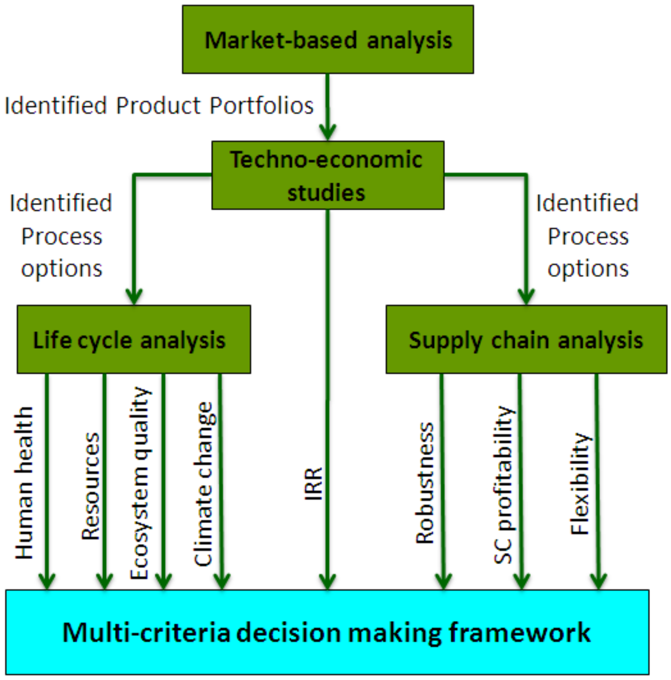

Fig. 7 - MCDM framework

Case Study Results and Discussion

In this section, an example is presented as an illustration. A P&P mill aims to implement FBR. The implemented biorefineries are decoupled biorefineries, meaning that no integration will exist between the biorefinery and the P&P. Thus, the mill should consider installing new processes, new inventories and new transportation system for the biorefinery.

Two product/process portfolios are considered. As shown in Fig. 7, market-based and techno-economic analyses have been used for this purpose and company corporate level decisions are crucial in this regard. The biomass to be used in both portfolios is a combination of wood chips, forest residues, sawmill residues, and hog fuel. In the first portfolio, Fischer-Tropsch liquids

(FTL) are produced by biomass gasification and a gas-to-liquid process, and then are separated into waxes (11000 U.S Gal/d) and diesel (13000 U.S Gal/d). Diesel can be converted into jet fuel (JF). The second portfolio involves production of succinic acid (SA) (195 Ton/d), malic acid (MA) (200 Ton/d) and lactic acid (LA) (150 Ton/d). All three products are produced in similar fermenters. SA and MA can be recovered in a similar recovery system, but LA needs a specific recovery system. Before fermentation, pre-treatment, extraction and hydrolysis processing steps are involved. SA and MA can be produced in one line, but in different production modes. Thus, the capacity presented for SA and MA belongs to the case when the whole capacity is dedicated to one of these two products. It is obvious that if both products are produced, the amount of each product will be smaller than the mentioned capacity.

The manufacturing processes are characterized in Table 2. This characterization helps to define design alternatives representing different flexibility potentials in the next step.

Portfolio	Characteristics
FTL to waxes and diesel+ diesel to JF	Type of process: Continuous Process configuration: Lines in series Product flexibility: Each line produces only one product Volume flexibility: Each process has 10% volume flexibility The share of waxes and diesel can change from 45%–55% to 55%–45%
SA MA LA	Type of process: Batch Process configuration: Lines in parallel Product flexibility: All products can be produced in similar fermenters, but in different modes. They need specific recovery systems Volume flexibility: Each process has 10% volume flexibility

Table 2 - Process characteristics for each product/process portfolio

Design alternatives representing different flexibility potentials for the portfolios are illustrated in Figure 8. The first portfolio is shown in Figure 8.a. In the first alternative, A-1, FTL is separated into waxes and diesel. The waxes are sold, and the whole diesel is converted to jet fuel (JF). In the second alternative, A-2, a smaller process is used to convert diesel to JF. Hence, this system has more potential for flexibility in terms of product. The third alternative is a combination of A-1 and A-2. Two small processes are used in parallel. If both are in operation, it performs like A-1 and if one of them is shut down, it performs like A-2. This alternative has the highest potential for flexibility.

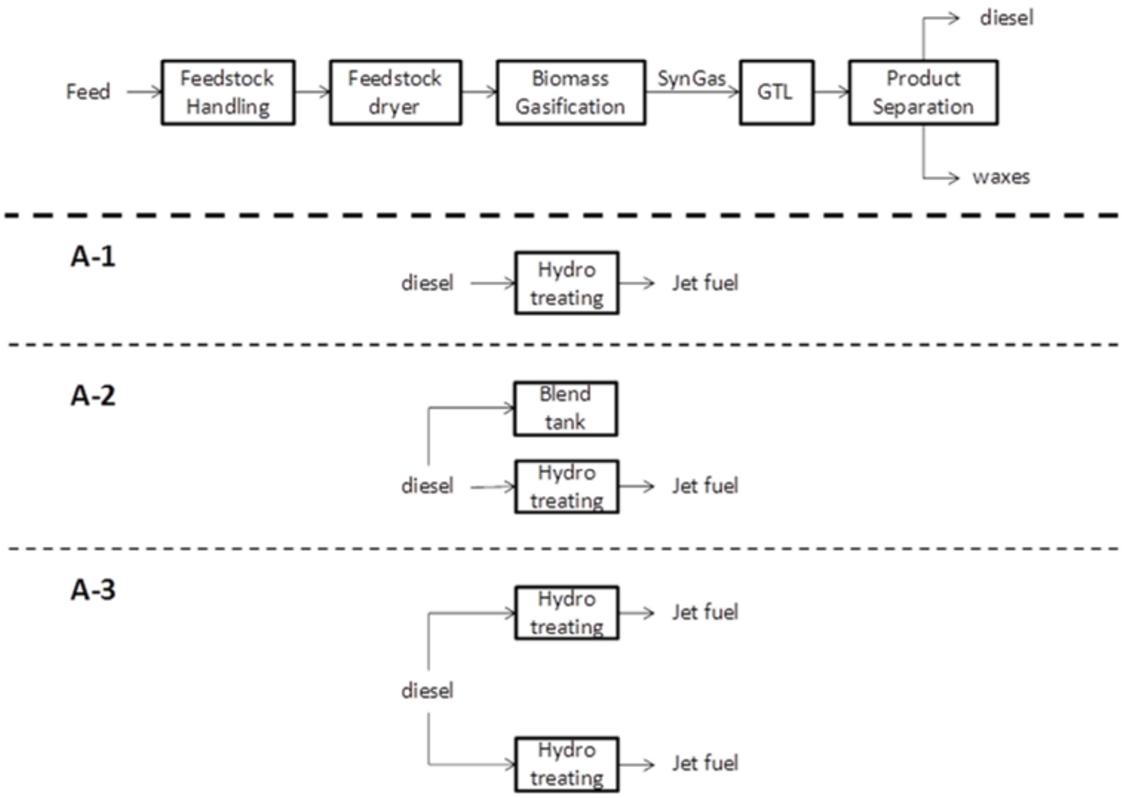

Fig. 8.a - Design alternatives for portfolio 1.

For the second portfolio, two design alternatives have been considered (Fig. 8.b). In the first alternative, B-1, there are two separate lines. The first line produces LA and the second line produces SA and MA in different production modes. In the second alternative, an SA/MA recovery system is added to the LA production line, so that this line can be changed over to produce SA or MA. One of SA/MA and LA recovery systems is always in standby mode. Hence, second alternative has more potential for flexibility.

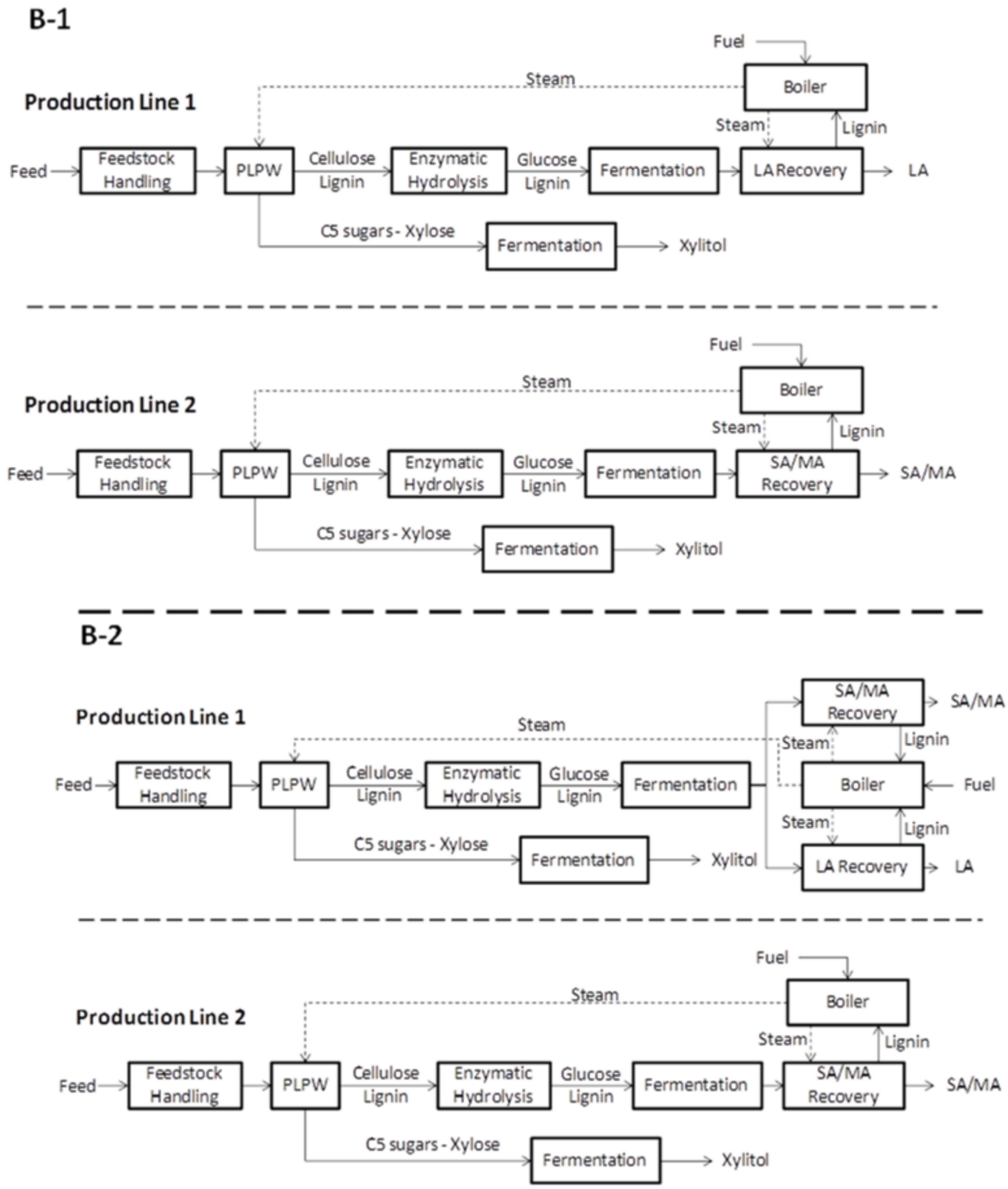

Fig. 8.b - Design alternatives for portfolio 2.

The capital investment required for each process in each portfolio is shown in Table 3.

Portfolio 1		Portfolio 2	
Design Alter.	Cap. Inv.($MM)	Design Alter.	Cap. Inv. ($MM)
A-1	138	B-1	104
A-2	120	B-2	106
A-3	146		

Table 3 - Capital investment needed for design alternatives

Tables 4 and 5 show the SC network alternatives defined for the each portfolio. Different transportation and selling strategies shown in these tables are defined by the mill's executives.

	SC network alternative for A-1	**SC network alternative for A-2**	**SC network alternative for A-3**
Selling	Waxes: Contract and spot Diesel: - Jet fuel: Contract	Waxes: Contract and spot Diesel: Spot Jet fuel: Contract	Waxes: Contract and spot Diesel: Spot Jet fuel: Contract and spot
Warehousing	Expansion	Expansion	Expansion
Transportation	Buy trucks	Contract with a transportation company	Contract with a transportation company

Table 4. SC network alternatives for portfolio 1

	SC network alternative for B-1	**SC network alternative for B-2**
Selling	SA: Contract and spot MA: Contract and spot LA: Contract and spot	SA: Possibility for more contract and spot MA: Contract and spot LA: Contract and spot
Warehousing	Expansion	More expansion
Transportation	Buy trucks	Contract with a transportation company

Table 5. SC network alternatives for portfolio 2

Market scenarios are shown in Fig. 9. Price and demand patterns are shown only for the second portfolio.

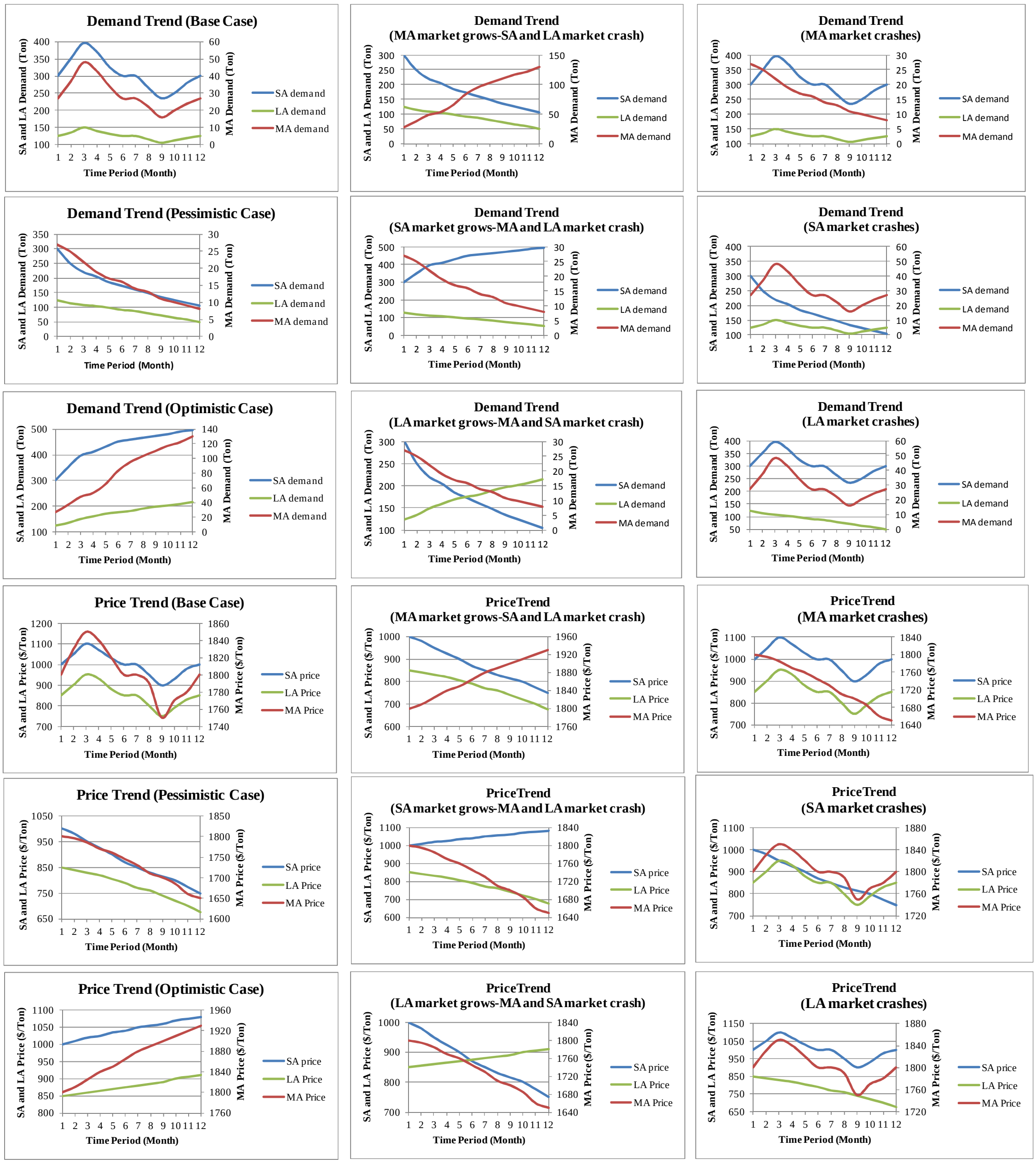

Fig. 9. Price and demand scenarios for case B.

SC optimization model is run for each alternative in case of all scenarios. The result of flexibility targeting step is shown for alternative B-1 in Figs. 10, 11 and 12. As can be observed in Fig. 10, profit improves with increasing flexibility up to 30%. Above 30%, the profit is not improved due to market conditions. Figure 11 illustrates the capital cost required for each flexibility level. From 0% to 24% volume flexibility, the increase in the capital cost is not significant, because the process has an inherent flexibility and with some slight modifications the level of flexibility is improved. In order to go beyond this level, major modifications are required to be done on the process, which incur more cost. Moreover, with more flexibility, more capacity will be available and the capital cost required for the SC will grow. As a result, the capital cost increases more sharply after 24% volume flexibility. The result of profitability (ROI) analysis is shown in Fig 12. Up to 24% flexibility, the increase in capital cost can be compensated by the profit improvements. In flexibility levels higher than 24%, the capital cost rise plays the major role and profit improvement in this range is not enough to pay off the extra capital cost. Hence, 24% can be targeted as the optimum level of flexibility.

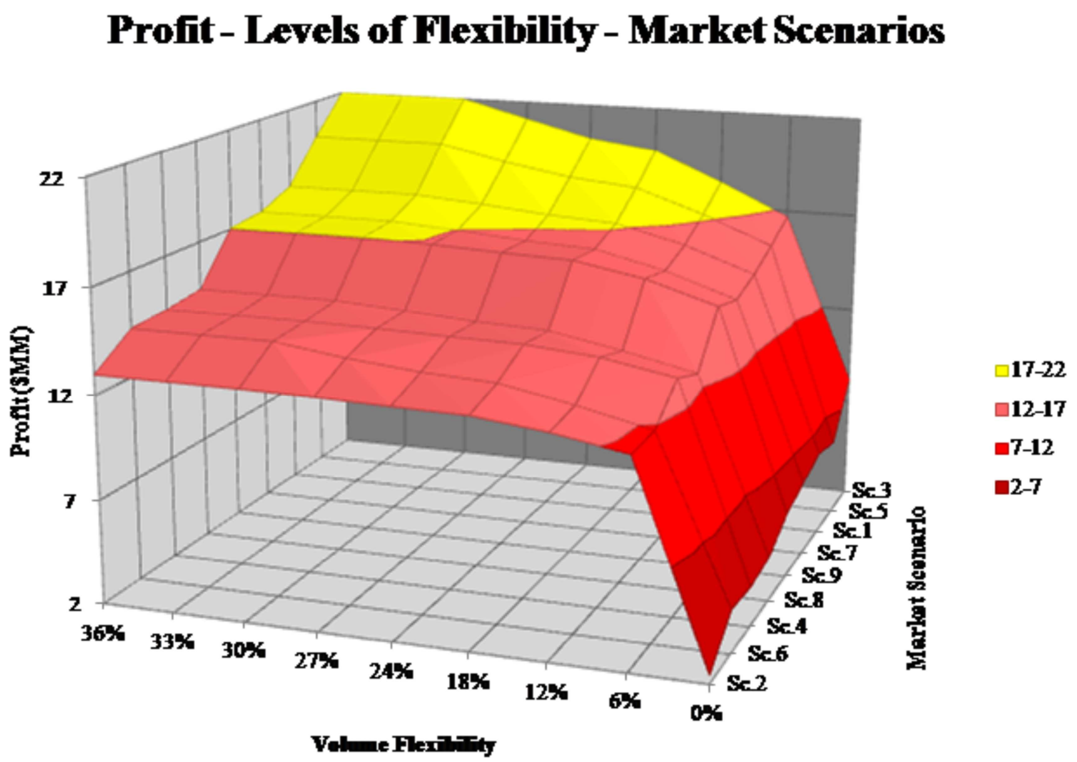

Fig. 10. SC profit of each level of flexibility in case of market scenario realizations; B-1.

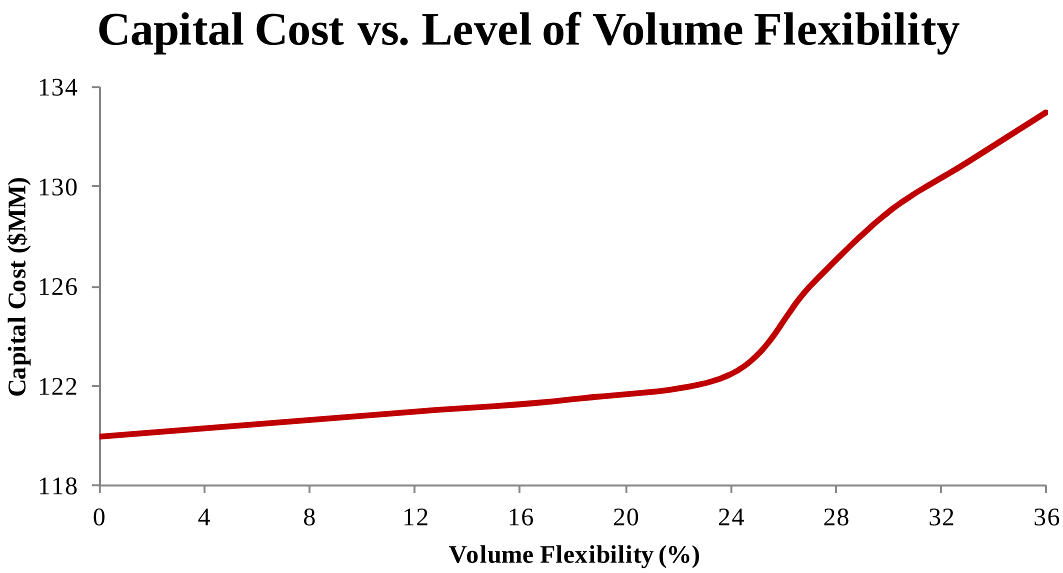

Fig. 11. Capital cost for levels of volume flexibility.

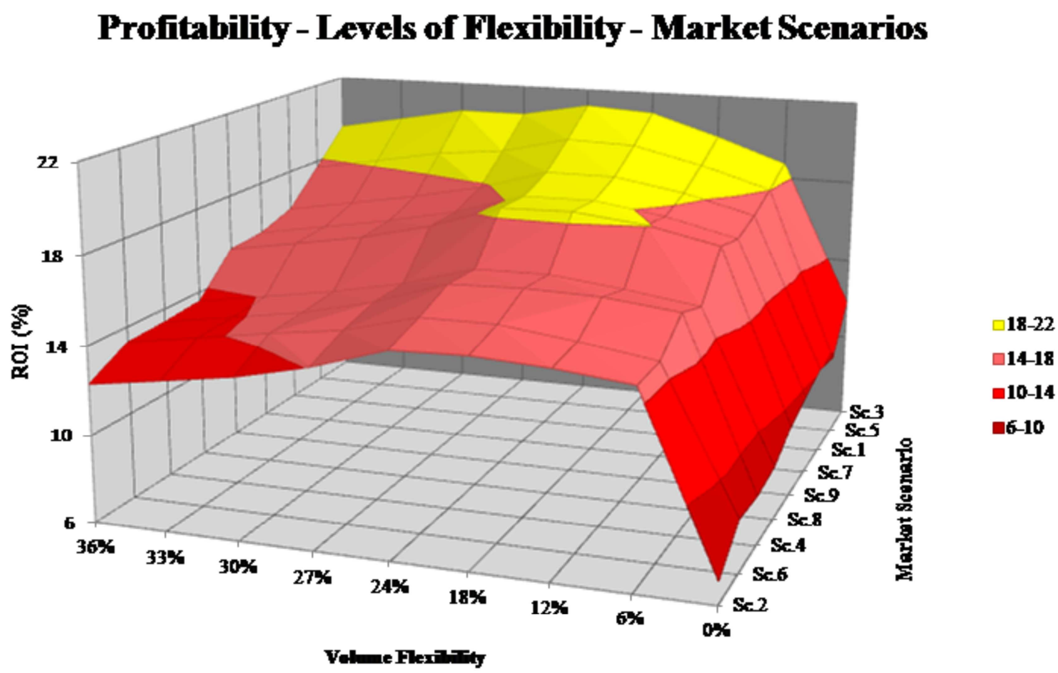

Fig. 12. Profitability of each level of flexibility in case of market scenario realizations.

SC profit, profitability, flexibility and robustness of each alternative are shown in table 6. As shown by the flexibility metric, as the potential for flexibility increases in each portfolio, more flexibility is used. Moreover, as more flexibility is used, profit increases and standard deviation

(SD) decreases, meaning that the SC is more robust against volatility. The first portfolio is not as sensitive as the second portfolio to volatility and the SD doesn't change significantly from one case to another. But in second portfolio, the change in SD is considerable. It can also be seen that more flexibility is used in the second portfolio and profitability is also higher compared to the first portfolio.

Another important observation is that the profitability does not necessarily increase with flexibility, because the increase in revenue cannot compensate the increase in capital and operating costs. It can be seen that profit increases with flexibility for all cases. But in case A, although A-3 is more flexible than A-2, its ROI is less. Second portfolio has a different behavior. Case B-2 leads to a higher profit and profitability compared to B-1. Thus, in can be concluded that, for this case, the extra capital spent for flexibility can very well be paid off.

Case	Profit/ Flexibility	Sc.1	Sc.2	Sc.3	Sc.4	Sc.5	Sc.6	Sc.7	Sc.8	Sc.9	Avg. Profit	ROI	Flexibility	SD ($MM)
A-1	Profit ($MM)	9.96	9.14	12.03	10.43	10.25	9.98	9.77	9.87	9.68	10.12	7.34%	12.67%	0.45
	Flexibility	8.18%	19.74%	16.58%	9.99%	8.62%	20.47%	12.95%	8.22%	9.28%				
A-2	Profit ($MM)	10.27	9.65	12.56	10.47	10.52	10.72	10.19	10.17	9.97	10.5	8.75%	17.36%	0.35
	Flexibility	9.54%	19.53%	38.72%	31.54%	33.16%	26.18%	8.29%	7.51%	8.34%				
A-3	Profit ($MM)	10.57	9.92	12.84	10.93	10.80	11.00	10.47	10.52	10.26	10.81	7.41%	19.46%	0.35
	Flexibility	16.44%	20.51%	39.05%	24.71%	6.63%	27.49%	8.29%	16.30%	15.71%				
B-1	Profit ($MM)	16.03	12.12	19.27	13.54	17.75	12.77	15.44	13.34	15.51	15.09	14.51%	25.13%	2.58
	Flexibility	24.69%	23.74%	28.69%	22.90%	27.33%	24.94%	24.95%	25.82%	23.10%				
B-2	Profit ($MM)	18.39	15.48	21.28	16.77	18.91	16.51	17.74	16.76	17.85	17.74	16.74%	30.20%	1.74
	Flexibility	32.38%	26.69%	34.52%	27.23%	32.70%	26.01%	33.20%	25.83%	33.26%				

Table 6. SC-related metrics for both cases.

A better insight about the problem will be given by scenarios generated for several years and a profitability metric that estimates the profitability of a project over the long term. Metrics such as internal rate of return can be more helpful in analyzing the effect of flexibility on the profitability of a project over the long run. It should be mentioned that the options can be implemented in several phases. For instance, option B-1 can be implemented and then a recovery system can be added to realize option B-2. Availability of capital for incremental investment over a period is of crucial importance in choosing options.

Conclusion

A hierarchical methodology is presented to incorporate flexibility design into SC design by integrating process design and SC design. The goal is to target the flexibility of several design alternatives by reflecting SC considerations into the design process. A scenario-based approach is applied in this methodology for addressing market volatility. An SC optimization model is used as a tool to calculate the profit of each alternative in case of all market scenarios, as well as other SC-related metrics, i.e. flexibility and robustness, that can be used to make the final decision. Such metrics can also be employed in an MCDM framework along with metrics provided by other analysis tools to make the final decision.

Acknowledgements

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APPENDIX D - Article: Scenario-based strategic supply chain design and analysis for the forest biorefinery

Scenario-Based Strategic Supply Chain Design and Analysis for the Forest Biorefinery Using an Operational Supply Chain Model

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Abstract

Supply chain (SC) design involves decisions for the long term, e.g. determining products, process technologies, number, location and capacity of different SC nodes, production rates, as well as suppliers, markets and partners. The forest biorefinery (FBR) is emerging as a new possibility for improving forestry companies' business models, however introduces significant technological, economic and financial challenges - which can be systematically addressed in strategic SC design. In order to reduce the burden of such challenges, partnership with companies whose expertise brings value and experience to the forestry companies' new business model is essential for FBR implementation. In this regard, redesigning the forestry SC in order for it to be aligned and consistent with the partner's SC, and in other words, designing a new integrated SC is of crucial importance.

This paper presents a scenario-based approach to strategic SC design for the FBR, designing the SC based on the impacts of the design on operational SC activities. Two kinds of scenarios are used; market scenarios representing market volatility and SC network scenarios (alternatives) representing different biorefinery options/strategies. In order to analyze the impacts of SC alternatives on operational activities, a *Margins-based* operational SC model examines the advantages and disadvantages of each scenario at this level by exploiting the capability of the SC for flexibility in the case of the market scenario realization. This demonstrates the impact of each scenario on SC profitability. It will also show how integration scenarios result in cost reductions

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compared to the case when the forestry company implements the biorefinery on its own and hence, it reveals how forestry companies can benefit from the created synergies.

Keywords: Forest Biorefinery, Supply Chain Design, Partnership, Scenario-Based Approach

1. Introduction

For a forestry company to improve its business model in the current market situation, it not only should diversify its revenue, but also must change its current manufacturing culture, which focuses on capacity management and neglects the profitability of the entire SC.

According to the strategic phased approach for the forest biorefinery (FBR) implementation shown in Fig. 1, revenue diversification will be achieved by means of "technology disruption" by producing building-block biorefinery chemicals, and ideally, in the longer term, by further increasing revenues by producing added-value derivatives. On the other side, manufacturing culture will be changed, in the short term, via "business disruption," through applying novel SC operating policies and exploiting production flexibility, and in the long term, by using advanced ERP and decision-making tools.

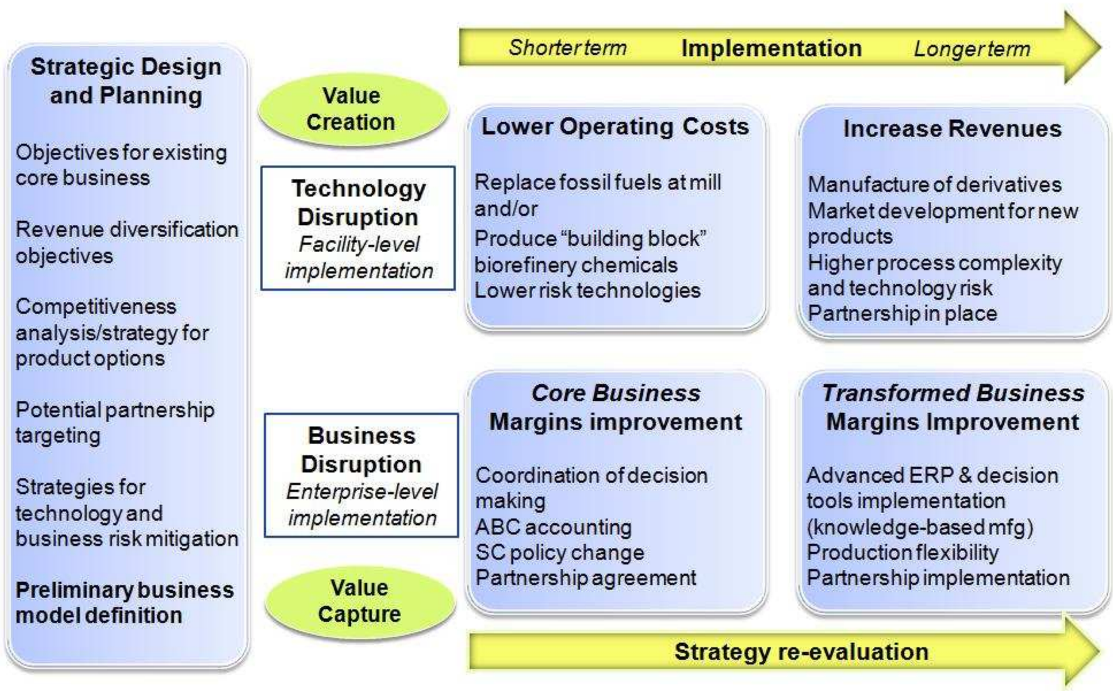

Fig. 1. Strategic implementation of the biorefinery by a forestry company.

SC analysis can play a key role in "business disruption". In the short term, to mitigate the risks of market volatility, companies should focus on improving their margins by implementing a *margins-based SC operating policy* and better exploiting the process capability for *flexible production* by using detailed knowledge of the process and its cost structure. Advanced SC optimization techniques can be used to carry out product planning over different time horizons and to identify tradeoffs between product orders and anticipated supply and demand. Over the long term, companies should base their strategic SC-related decisions on a bottom-up approach, i.e. designing/redesigning the SC based on the impact of the design on tactical and operational activities. These two approaches to the short-term and long-term aspects of biorefinery implementation, i.e. the margins-based approach and the bottom-up approach, imply profound changes in the way forestry companies do business today, which is equivalent to business disruption.

In the design of a SC, strategic long-term decisions should be made, i.e. products, technologies, number, location and capacity of each facility, e.g. plants, warehouses and distribution centres, and the target markets. As a result, SC-based analyses that address long-term decisions are used as a tool for analyzing and evaluating long-term strategies. Application of SC-based analysis in biorefinery design decision making is getting attention. Sammons et al. (2008) proposed a general systematic framework for optimizing product portfolio and process configuration in integrated biorefineries. The framework first determines the variable costs as well as fixed costs using data in terms of yield, conversion and energy usage for each process model. Next, process integration tools, e.g. pinch analysis, are employed to optimize the models. Finally, the optimized model will generate data for economic and environmental performance metrics. An optimization formulation enables the framework to decide whether a certain product should be sold or processed further, or which processing route to pursue if multiple production pathways exist for a special product. Tursun et al. (2008) developed a mathematical programming model that determines optimal locations and capacities of biorefineries, delivery of bioenergy crops to biorefineries, and processing and distribution of ethanol and co-products across Illinois. Slade et al. (2009) analyzed the role of SC design on the viability of commercial cellulosic ethanol projects in Europe. They showed how an SC-based analysis can shed light on the major cost contributors in a project. Eksioglu et al. (2009) developed a mathematical model to analyze and manage a biomass-to-biorefinery SC. Mansoornejad et al. (2010) develop a systematic hierarchical methodology to integrate product portfolio design with SC network design in the FBR. Separate methodologies for product portfolio definition, process technology selection, and SC design are integrated in the proposed hierarchical methodology. It is described how these methodologies along with other analysis tools such as life cycle analysis (LCA) can provide metrics and criteria to be used in a multi-criteria decision-making (MCDM) framework for making the final decision. Huang et al. (2010) introduce a process model to simulate an integrated FBR manufacturing pulp and other co-products. The model has been used to compare three alternatives: the conventional Kraft pulping process, the pulp mill integrated with hemicelluloses extraction prior to pulping for ethanol production, and the pulp mill integrated with both pre-extracted hemicelluloses and the short fiber for ethanol production. Sharma et al. (2011) introduce a model for assessing the impact of feedstock and technology selection, process and utility integration, and effluent recycle for a multi product multi platform biorefining enterprise. Mele et al. (2011) develop a multi-objective mixed integer linear programming (MILP) that is used as a quantitative tool to support SC design decision-making and aims at optimizing the economic and environmental performance of a combined sugar and ethanol production chain. Kim et al. (2011) present a model for the optimal design of biomass SC networks under uncertainty, covering an SC located in the Southeastern region of the United States. The SC consists of biomass supply locations and amounts, candidate sites and capacities for two kinds of fuel conversion processing, and the logistics of transportation from the locations of forestry resources to the conversion sites and then to the final markets. A two stage stochastic approach is used to solve the MILP with the objective of maximizing the expected profit over the different scenarios. The robustness and global sensitivity analysis of the nominal design (for a single nominal scenario) vs. the robust design (for multiple scenarios) are analyzed using Monte Carlo simulation. Giarola et al. (2011) present an MILP framework for the strategic design and planning of corn grain and stover-based bioethanol SCs through first and second generation technologies, which optimizes the environmental and financial performances simultaneously. Bowling et al. (2011) introduce a systematic approach for the optimal production planning and facility placement of a biorefinery using an optimization formulation which specifically determines the optimal SC, size, operational strategies, location of the biorefinery and pre-processing hub facilities, and selection of biomass to maximize overall net profit. The model takes into account non-linear economy-of-scale behavior of the capital cost functions that are reformulated using disjunctive models to yield convex relationships to guarantee a global optimal solution. Marvin et al. (2012) study the NPV of a biomass-to-ethanol supply chain in a 9-state region in the Midwestern United States, using an MILP to find optimal locations and capacities of biorefineries in conjunction with biomass harvest and distribution. Monte Carlo simulation is performed to investigate the robustness of the SC and whether or not the proposed biorefineries will be built or will fail financially after being built.

The decision as to what biorefinery strategy to take depends on many factors, most of which cannot be reflected in an optimization problem, e.g., understanding the market and market strategies, emerging products and technologies, the capabilities of existing SC assets, and potential partners. In a practical problem, it is difficult to address all these decision variables within a single SC optimization model. Instead, it is preferable to pursue a systematic hierarchical methodology that addresses all these factors in a stepwise manner. Because of the combinatorial aspect of such design problems, the hierarchical methodology might miss the global optimum. However, such a methodology does not seek to identify a global optimum. Rather, it seeks a set of feasible and practical biorefinery options that a company can strategically pursue. Many of the key aspects can be addressed in different scenarios instead of being modeled into an optimization formulation. In this way, a simpler model will be solved, with more practical results. This methodology would end up with a set of solutions. An MCDM framework can be used to find the best option from a specific company's point of view.

In order to execute this hierarchical methodology, certain decisions must be made via integration with other methodologies. To achieve a hierarchical methodology, some of these decisions must be made by integration with other methodologies. The set of products is identified by a product portfolio definition/selection methodology. The processes and technologies are chosen through a techno-economic study. What will be determined by the scenario-based SC design is the SC network design including the number, location and capacity of warehouses, target customers, types of orders to fulfil, i.e. contract or spot, as well as partners to collaborate with.

This paper introduces a scenario-based approach for the design and analysis of SCs for the FBR using a stepwise methodology that aims at reflecting the practical aspects of design into decision making. The stepwise methodology utilizes an operational SC model to analyze the impact of design decisions on the operational level activities. SC performance metrics are introduced to quantify the performance of each design alternative at the operational level.

The rest of the paper is organized as follows. First, the problem and key concepts used in this paper is explained. Then, the SC optimization framework is discussed. Afterwards, the proposed methodology for SC-based analysis is presented and discussed along with a case study to concretize the methodology. Finally, some concluding remarks are drawn.

2. Problem definition

A forestry company plans to implement the biorefinery by examining the portfolio of products which secure profit, using processes which enable better response to volatile market conditions, and companies with which a partnership can be made. On one hand, market volatility must be taken into consideration, and on the other hand, possible product/process/SC network options to be implemented must be identified. Scenario generation is used to address both aspects. Market conditions are reflected into the problem via market scenarios. Also, possible biorefinery options, each implying a specific implementation strategy, are made in terms of alternatives, each of which includes (1) a product portfolio, (2) a technology for the production of each product, and (3) a SC network for each portfolio. Given are a set of product portfolios and a set of process technologies that can be used to produce those products with known capital and operating cost. SC network alternatives are defined and combined with product/process portfolios. A margins-based SC optimization model is used to calculate the profit of each combined alternative in case of several market conditions. Several market scenarios, including product price and demand change over a period of one year, are also defined as the input to the problem to represent market volatility. The SC model calculates the profitability and quantifies the flexibility of each combined alternative in case of market scenario realizations. Moreover, robustness of the SC against all market scenarios is quantified using the calculated profits.

The SC network must be designed in a way such that, by optimizing the operational SC activities, SC profit is maximized. As a result, this approach evaluates the SC network design based on the impacts of the design on operational activities. The margins-based optimization model takes advantage of the flexibility of processes, and chooses orders and plans production so that profit is maximized. In the following sections, key concepts used in this article, i.e. margins-based operating policy, manufacturing flexibility and partnership, are discussed.

2.1. *Margins-based operating policy*

The operating policy in the P&P industry is said to be “manufacturing-centric.” In this industrial sector, the management focus is on capacity planning, and industry participants try to achieve the efficient and effective use of machine capacity (Lail, 2003). As a result, process efficiency is viewed as the key measure for profitability, and therefore it is believed that minimizing production cost will result in the highest profitability (Dansereau et al., 2009). Moreover, production planning assumes a known set of orders and a fixed sequence of product grades. By treating the manufacturing process as the focal point, inventory and changeover costs are typically ignored or considered separately (Lail, 2003), and SC costs are often neglected, resulting in lower profitability (Dansereau et al., 2009).

To implement the FBR, the operating policy must shift from a manufacturing-centric approach to a margins-based one. This latter operating policy tries to maximize margins over the entire SC and to produce and select products and orders that ensure the best returns (Dansereau et al., 2009). In this approach, long-term contracts and short-term order selection is made with respect, not only to process and production constraints, but to all SC constraints, including for example inventory and transportation constraints, to maximize the ultimate SC profitability.

2.2. *Manufacturing flexibility*

Today’s market is subject to huge volatilities in terms of price and demand. The price of oil, fuels, and chemicals, as well as the price of forestry products, change even on a monthly basis. The demand for some products is not always certain, and sometimes, despite strong demand, the price is too low for the production of a product to be profitable. On the feedstock side, uncertainty exists in terms of price and availability. A forestry company might be obliged to procure its feedstock from different sources over different distances and with different prices (Eksioglu et al., 2009). Short product life cycles and increasing competition among companies reveal new uncertainties and risks for different industries. All these clauses entail more uncertainty and risk for the companies. To mitigate risks in the face of such uncertainties, it is of crucial importance to enhance adaptiveness and reactivity on one hand and proactivity on the other hand (Schiltknecht & Reimann, 2009). These capabilities are generally called *flexibility*. Based on the type of uncertainty and how it is addressed, there are different types of flexibility, which will be discussed later in this paper.

An FBR would be exposed to this kind of volatile environment and would face these risks and uncertainties. Hence, flexibility, of any possible type, must be exploited in an FBR to mitigate risks. An FBR will be able to produce several products, including P&P products, bioproducts, and energy. Producing several products implies the opportunity to take advantage of manufacturing flexibility, i.e., producing different products at different volumes in different time periods. In a volatile market, depending on feedstock and product prices as well as supply and demand, manufacturing flexibility can be exploited, and the mill can produce different products in different amounts to optimize and secure the company's margin. The company should analyze its access to feedstocks, product prices, and received as well as forecasted demands and find the best alignment between these demands and its production capacity to maximize the company's profit.

The concept of manufacturing flexibility in the FBR implies the ability to produce several bioproducts at different volumes and in different time periods based on product price and demand. This definition is an aggregation of product flexibility and volume flexibility. Manufacturing flexibility implies a justifiable increase in capital and operating cost that is adequately compensated by the ability of the process to manufacture in a flexible manner so that the expected volatility in market conditions can be mitigated.

2.3. *Partnership*

Partnership is defined as companies in different industries with different but complementary skills which link their capabilities to create value for ultimate users (Kanter, 1994). Generic advantages of making partnership include (a) accessing complementary assets and know-how, (b) reducing time to market, and (c) sharing investment costs (Kanter, 1994). Given the characteristics of the FBR implementation, specific advantages for the FBR are (a) meeting profitability targets, (b) reducing transformation risks of new products, (c) ensuring rapid and efficient business development ahead of other competitors, (d) entering an existing value chain, and (e) efficiently setting up delivery systems (Janssen et al., 2008).

In the FBR partnership can be made with feedstock partners, who will increase supply and decrease cost, commercial partners, who can help in product development and delivery to the market, technology partners, who provide the technology, and financial partners, who supports the company financially and benefit from the increased potential profitability (Janssen et al., 2008). Several partnerships have been made thus far in the context of biorefinery. UPM-Kymmene & Andritz-Carbona made a strategic partnership on the development of a technology for biomass gasification and biodeisel production. Weyerhaeuser & Chevron created a joint venture (JV) called Catchlight Energy LLC, whose goal is to develop economical low-carbon biofuels. StoraEnso & Neste Oil made a 50/50 JV for developing technology for biofuel production from wood residues. In the JV, StoraEnso supplies woody biomass and produces biofuel and is responsible for the heat generated at its mills, while Neste Oil will do the final refining and marketing of biofuel (chambost et al., 2009).

Critical elements that must be addressed in creating partnership are the strategic compatibility of business models and visions, the long-term capital investments required, and the potential revenue diversification (chambost et al., 2009).

3. SC performance metrics

As stated by Beamon (1998), establishment of appropriate performance measures is an important component in SC design and analysis. Performance measures can be used either in comparing competing alternative systems, or in designing proposed systems, by determining the values of the decision variables that yield the most desirable level(s) of performance. These measures can be classified into two categories; qualitative and quantitative. Qualitative performance measures are those measures for which there is no single direct numerical measurement, although some aspects of them may be quantified. Customer satisfaction, flexibility, information and material flow integration, effective risk management, supplier performance are example of qualitative measures. On the other hand, quantitative performance measures may be defined numerically. Such measures may be described by, either objectives that are based directly on cost or profit such as cost minimization, sales maximization, profit maximization, inventory investment minimization, return on investment maximization, or objectives that are based on some measure of customer responsiveness like fill rate maximization, product lateness minimization, customer response time minimization, lead time minimization, function duplication minimization.

In this work, two metrics are used to evaluate the performance of SC in volatile market; metric of flexibility (MF) and metric of robustness (MR). These metrics are not part of the decision variables of the SC model, and thus, they are not optimized. They are just calculated and used to quantify the flexibility and robustness of SC in volatile market conditions.

3.1. *Metric of flexibility (MF)*

Beamon (1998) defined the measure of flexibility as the degree to which the supply chain can respond to random fluctuations in the demand pattern. This is a generic definition and involves all types of flexibility. In systems engineering, many works are done on the issue of flexibility based on the work of Swaney and Grossmann (1985). They defined flexibility index as a metric that characterizes the size of the region of feasible operation in the uncertain parameter space. Another measure of flexibility was introduced by Voudouris (1996) which defines flexibility as the ability of the system to absorb unexpected demand.

In this paper, a metric of flexibility is presented that can be well applied for design purposes for the FBR design. In the design of chemical processes, volume flexibility has a critical role. Thus, in order to design or analyse the flexibility of a system, quantifying volume flexibility is of crucial importance. Inspired by the work of Voudouris (1996) on qualitative measure of flexibility, metric of flexibility (MF) quantifies volume flexibility, as shown in equation 1:

$$MF = \sum_t \sum_p \sum_m \left| \frac{C_{mpt} - C_{mp}^N}{C_{mp}^N} \right| \quad (1)$$

where $\mathrm{C_{mpt}}$ is the amount of product m that is produced on process p in time period t and $\mathrm{C_{mp}^N}$ is the amount of product m produced on process p by the nominal production rate over the same number of processing hours. This formulation shows the deviation from the nominal production rate in a dimensionless form and implies volume flexibility.

3.2. *Metric of robustness (MR)*

In a robust design the control parameters of a system are selected in such a way that the desirable measured function do not diverge significantly from a given value (Bernardo, Pistikopoulos, & Saraiva, 1999). In this work, robustness is not considered in the optimization formulation. Instead, a metric of robustness (MF) is used to quantify the robustness of design options against market volatility so that design options can be compared in terms of robustness. Several robustness metrics have been introduced thus far (Vin & Ierapetritou, 2001). Well-known metrics are standard deviation and mean absolute deviation (Bernardo, Pistikopoulos, &

Saraiva, 2001). For the sake of simplicity and interpretability for an MCDM panel, we use a simple formulation as robustness metric, as shown in equation 2.

$$\mathrm{MR} = \left(\frac{\sum_{\mathrm{Sc}}(\mathrm{Pr_B} - \mathrm{Pr_{Sc}})}{\mathrm{Pr_B}}\right)^{-1} \qquad (2)$$

where $\mathrm{Pr_B}$ is the base case profit, $\mathrm{Pr_{Sc}}$ is the profit for scenario Sc and $\mathrm{N_{Sc}}$ is the number of scenarios. In this work, the desired parameter that must not diverge from a given value is profit. It is desirable that the profit of a design option in case of each market scenario does not deviate from the base case profit, if this profit is lower than the base case profit, i.e. a downside profit. Therefore, to quantify the downside risk of volatility, the downside profits are considered in this equation. The MR shows the percentage of aggregate deviation from the base case profit for all downside profits. The smaller this percentage is the better and more robust the system is. Hence, the reverse of the percentage was used so that the higher values of MR represent more robust systems.

4. SC optimization framework

Fig. 2 illustrates the SC of an FBR. Several types of feedstock, ranging from forest biomass to recycled papers and agricultural residues, can be used. Feedstock is treated and prepared to be used in the plants. The final products involve wood and paper products, biofuel, green chemicals and energy.

There is a strong body of knowledge related to SC mathematical formulation. Such formulations address strategic design, tactical planning or operational and scheduling SC decisions. Some examples can be viewed in Voudouris (1996), Timpe and Kallrath (2000), Jin-Kwang, Grossmann, and Park (2000), Tsiakis, Shah, and Pantelides (2001), Sousa, Shah, and Papageorgiou (2005), and You and Grossmann (2008).

The SC framework aims at maximizing profit across the entire SC by identifying the tradeoffs between demand and production capabilities and by finding the optimal alignment of manufacturing capacity and market demand. The SC optimization framework considers feedstock price and availability, production costs, and inventory and delivery costs, as well as product price and demand. Taking this information into account, the SC optimization framework will exploit the potential for production flexibility and determine which orders must be fulfilled and therefore how much of which products must be produced, how they should be stored, and how they should be delivered to the market to maximize SC profit.

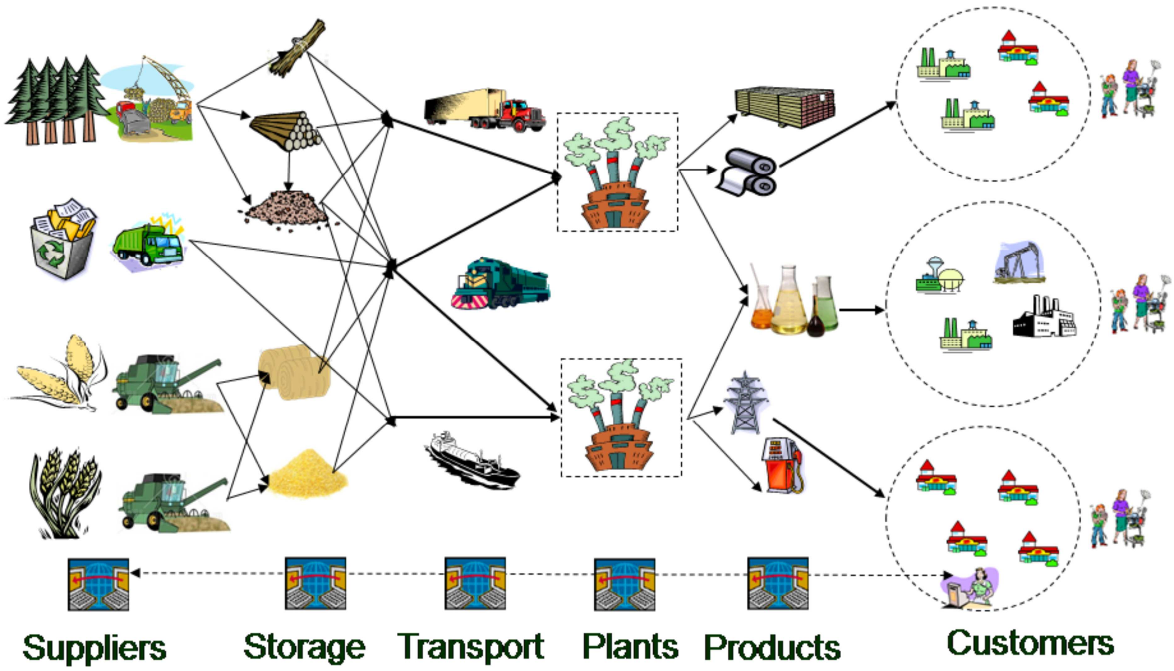

Fig. 2. Forest biorefinery supply chain.

4.1. *Executing the margins-based policy*

As mentioned earlier, what drives the margins-based policy is the ultimate profitability of the entire SC. All SC activities must be executed with respect to this policy. In the forestry industry, especially in the P&P sector, some SC practices are contrary to this approach. One of the most important of these practices is treating production cost as the major driver in decision-making. In this way, operating cost is generally used as the objective function, and the costs incurred by other nodes of the SC are basically neglected (Lail, 2003). Therefore, the first point to be made in an SC optimization framework with a margins-based policy is that profit must be used as the objective function.

Another common practice in the forestry industry is that products are produced in fixed known sequences and the capability of the process for flexibililty in production and changeover is not used (Dansereau et al., 2009). This can result in decreasing the profitability of the company when prices or demands change. Suppose that, based on the established sequences, the company has produced some products that in a particular period, are subject to low price or weak demand. In the case of weak demand, the company should store its products for a longer period, in which case the inventory cost rises. In such a case, the company might sell its products at a discount, which would decrease the profit. Moreover, some companies take orders based on their sequences, and they miss out on better orders just because these orders do not fit their production sequence. Hence, another point that must be respected in an SC optimization framework with a margins-based policy is to let the framework choose the best orders and to take advantage of the mill's capability of flexibility and changeover, leaving aside traditional recipes and practices.

4.2. *SC optimization framework*

It is desirable to account for tactical and operational issues at the strategic design level. On the other hand, for design purposes, it is not necessary to go down to too much details, as provided by scheduling models. For this reason, the SC framework that is presented in this work is inspired by the tactical model developed for the chemical industry by Kanegiesser (2008). This model is a tactical model that has some operational components. The model divides each time period into several hours that can be dedicated to production, changeover or maintenance. In this way, a better cost representation can be made by the model.

The SC framework is formulated as an optimization problem with the objective of maximizing profit. This framework considers the management of a multi-product, multi-echelon SC, including existing production and warehousing facilities as well as a number of customer zones, although it can also be used for design purposes. Different types of biomass are provided by several suppliers. Production facilities can make one or several products. Processes are either dedicated, i.e. they produce only one product, or flexible from a product perspective, i.e. they are able to produce several products through different recipes. In other words, a flexible process can use different recipes to produce different products. Changing from one recipe to another incurs changeover cost and time. Processes can be idled or shutdown for scheduled maintenance. The steam required for each process is provided by both fuel and biomass. Warehouses can receive material, either feedstock or product, from different sources and plants, and supply different markets. Each market places demand in two ways: by contract, i.e., for the long term, and in the spot market, i.e., for the short term. In case of a contract, specific quantities of products must be sold to the customer in specific time periods. The spot demand can be partially fulfilled. Transportation routes link suppliers, facilities and customers together. The model is formulated as an MILP problem with a discrete time horizon of 48 weeks. Each time period is broken down into hours. Several subsets have been created to link parameters and variables to each other. For instance, some customers will only accept products from specific mills. Processes can only produce certain materials. This will reduce the possible options and thus, the complexity of the problem. The model is presented below:

Nomenclature

Sets

$j \in J$	Supplier locations
$l \in L$	Mill locations
$k \in K$	Sales locations
$p \in P$	Processes
$r \in R$	Recipes
$m \in M$	Materials
$t \in T$	Time

Subsets

Suppliers that can supply mill: $\{j,l\} \in L^{JL} \quad \forall j \in J, l \in L$

Customers that can be served by mill $\{l,k\} \in L^{LK} \quad \forall l \in L, k \in K$

Processes at mill $\{l,p\} \in P^{L} \quad \forall l \in L, p \in P$

Recipes available on process $\{l,p,r\} \in R^{P} \quad \forall \{l,p\} \in P^{L}, r \in R$

Materials offered by suppliers $\{j,m\} \in M^{J} \quad \forall j \in J, m \in M$

Materials produced/processed at mill $\{l,m\} \in M^{L} \quad \forall l \in L, m \in M$

Materials requested by customers $\{k,m\} \in M^{K} \quad \forall k \in K, m \in M$

Input materials of a process $\{l,p,m\} \in M^{P-in} \quad \forall \{l,p\} \in P^{L}, m \in M$

Output materials of a process $\{l,p,m\} \in M^{P-out} \quad \forall \{l,p\} \in P^{L}, m \in M$

Input materials of a recipe $\{l,p,r,m\} \in M^{R-in} \quad \forall \{l,p,r\} \in R^{P}, m \in M$

Output materials of a recipe $\{l,p,r,m\} \in M^{R-out} \quad \forall \{l,p,r\} \in R^P, m \in M$

Constructed Subsets

Materials that can be transported between a supplier and a mill:

$\{j,l,m\} \in M^{JL} \quad \forall \{j,l\} \in L^{JL}, \{j,m\} \in M^J, \{l,m\} \in M^L$

Materials that can be transported between a mill and a customer:

$\{l,k,m\} \in M^{LK} \quad \forall \{l,k\} \in L^{LK}, \{l,m\} \in M^L, \{k,m\} \in M^K$

Parameters

a_{lprm}^{input} Recipe material conversion Input factor of material m when using recipe r on process *p* in mill *l* (dependent on throughput)

a_{lprm}^{output} Output factor of material *m* when using recipe *r* on process *p* in mill *l*

$b_{lpr}^{input-steam}$ Steam consumption factor for recipe *r* in process *p* in mill *l*

$b_{lpr}^{output-steam}$ Steam production factor for recipe *r* in process *p* in mill *l*

$b_{lpr}^{input-elect}$ Electricity consumption factor for recipe *r* in process *p* in mill *l*

$b_{lpr}^{output-elect}$ Electricity production factor for recipe *r* in process *p* in mill *l*

$c_{lpr}^{proc-var}$ Variable operating cost of using recipe r on process p in mill l (dependent on process throughput)

$c_{lt}^{mill-fix}$ Fixed operating cost at mill *l* during time period *t*

$c_{jlm}^{transport-sup}$ Transportation cost of material *m* from supplier *j* to mill *l*

$c_{lkm}^{transport-sales}$ Transportation cost of material *m* from mill *l* to a customer *k*

c_{lm}^{stor} Storage cost of material *m* in mill *l*

$c_{lp}^{shutdown}$ Shutdown cost of process *p* in mill *l*

$c_{lp}^{changeover}$ Changeover cost of process *p* in mill *l*

c_{lt}^{elect} Electricity cost / selling price at mill *l* during time period *t*

c_{kmt}^{sales} Selling price of product *m* to customer *k* during time period *t*

c_{jmt}^{sup} Purchasing price of a feedstock *m* from supplier *j* during time period *t*

$c_{kmt}^{salescost}$ Sales cost for product *m* sold to customer *k* during time period *t*

H_{lpr}^{camp} Minimum campaign length for recipe *r* in process *p* in mill *l*

$H_{lp}^{changeover}$ Changeover time on process *p* in mill *l*

H_{lpt}^{proc} Available processing hours on process *p* in mill *l* during time period *t*

$\underline{Q}_{lpr}^{proc}$ Minimum throughput (process rate) of recipe *r* on process *p* in mill *l*

$\overline{Q}_{lpr}^{proc}$ Maximum throughput (process rate) of recipe *r* on process *p* in mill *l*

$\underline{Q}_{lm}^{stor}$ Minimum storage quantity of material *m* in mill *l*

$\overline{Q}_{lm}^{stor}$ Maximum storage quantity of material *m* in mill *l*

$\underline{Q}_{jmt}^{supp}$ Minimum supply quantity of material *m* offered by supplier *j* during time period *t*

$\overline{Q}_{jmt}^{supp}$ Maximum supply quantity of material *m* offered by supplier *j* during time period *t*

$\underline{Q}_{kmt}^{sales}$ Minimum quantity of material *m* requested by customer *k* during time period *t*

$\overline{Q}_{kmt}^{sales}$ Maximum quantity of material *m* requested by customer *k* during time period *t*

$\overline{Q}_{jlm}^{transport}$ Maximum transportation quantity of material *m* between supplier *j* and mill *l*

$\overline{Q}_{lkm}^{transport}$ Maximum transportation quantity of material *m* between customer *k* and mill *l*

$S_{lm}^{mat-start}$ Initial storage quantity of material *m* in mill *l* at time 0

$S_{lm}^{mat-end}$ Minimum storage quantity of material *m* in mill *l* at time T

ε_{lpt}^{proc} Shutdown hours on process *p* in mill *l* during time period *t*

$\alpha_{lpr}^{rec-start}$ Initial recipe *r* on process *p* in mill *l*

Variables

f_{jlmt}^{sup} Flow of material *m* from supplier *j* to mill *l* during time period *t*

f_{lkmt}^{mill} Flow of material *m* from mill *l* to customer *k* during time period *t*

h_{lprt}^{rec} Number of hours spent on recipe *r* on process *p* in mill *l* during time period *t*

S_{lmt}^{mat} Inventory of material *m* in mill *l* during time period *t*

v_{lpt}^{input} Input steam quantity on process *p* in mill *l* during time period *t*

v_{lpt}^{output} Output steam quantity on process *p* in mill *l* during time period *t*

w_{lpt}^{input}	Input electricity quantity on process *p* in mill *l* during time period *t*
w_{lpt}^{output}	Output electricity quantity on process *p* in mill *l* during time period *t*
x_{lmpt}^{proc}	Input quantity of material m on process *p* in mill *l* during time period *t*
y_{lmpt}^{proc}	Output quantity of material m on process *p* in mill *l* during time period *t*
y_{lprmt}^{rec}	Output quantity of material m using recipe *r* on process *p* in mill *l* during time period *t*
$y_{lprt}^{rec-tot}$	Total mass output of recipe *r* on process *p* in mill *l* during time period *t*
α_{lprt}^{proc}	Selection of recipe *r* on process *p* in mill *l* during time period *t* (binary)
β_{lprt}^{proc}	Successive selection of recipe *r* on process *p* in mill *l* during time periods *t* and *t-1* (binary)
θ_{kmt}^{ord}	Selection of the order of product *m* from customer *k* during time period *t* (binary)

Objective Function

The objective function is the global net profit of the enterprise to be maximized. This profit consists of revenues from the sales of products and electricity, minus several variable and fixed costs.

$$\max Profit = \begin{pmatrix} Revenues - ElectricityCost - SalesCost \\ -VariableOpCost - FixedOpCost - ChangeoverCost - ShutdownCost \\ -TransportationCost - StorageCost - ProcurementCost \end{pmatrix} \tag{3}$$

Revenues from sales are equal to the flow of materials sent to each customer multiplied by the selling price.

$$Revenue = \sum_{t\in T} \sum_{\{k,m\}\in M^K} f_{lkmt}^{sales} c_{kmt}^{sales} \tag{4}$$

Electricity sales or purchases are function of the production/consumption at the mill. If the mill produces more electricity than needed, then electricity is sold to the grid. Otherwise, it is assumed it is bought from the grid at the same price.

$$ElectricityCost = \sum_{t\in T} \sum_{\{l,p\}\in P^L} (w_{lpt}^{input} - w_{lpt}^{output}) c_{lt}^{elect} \tag{5}$$

Variable sales costs are customer specific and are a percentage of product prices.

$$SalesCost = \sum_{t\in T} \sum_{\{k,m\}\in M^K} f_{lkmt}^{sales} c_{kmt}^{salescost} \tag{6}$$

Variable operating costs are a function of process throughput such as chemical consumption.

$$VariableOpCost = \sum_{t \in T} \sum_{\{l,p,r\} \in R^P} c_{lpr}^{proc-var} y_{lprt}^{rec-total} \tag{7}$$

Fixed operating costs are calculated at the plant.

$$FixedOpCost = \sum_{t \in T} \sum_{l \in L^{mill}} c_{lt}^{mill-fix} \tag{8}$$

Changeover cost is equal to the number of transitions multiplied by the changeover cost per transition. This cost is not considered sequence dependent.

$$ChangeoverCost = \sum_{t \in T} \sum_{\{l,p,r\} \in R^P} (1 - \sum_{r \in R_p^{proc}} \beta_{lprt}^{proc})\, c_{lp}^{changeover} \tag{9}$$

The shutdown cost of a process is a function of the number of shutdown hours during a time period. Scheduled shutdowns for maintenance are considered here as a hard constraint.

$$ShutdownCost = \sum_{t \in T} \sum_{\{l,p\} \in P^L} \varepsilon_{pt}^{proc} c_{lp}^{shutdown} \tag{10}$$

Transportation cost is calculated by multiplying the amount of material shipped from a source (supplier *j* or mill l) to a sink (mill *l* or customer *k*) and the shipping cost per mass of that route.

$$TransportationCost = \sum_{t \in T} \sum_{\{j,l,m\} \in M^{JL}} f_{jlmt}^{sup} c_{jlm}^{transport-sup} + \sum_{t \in T} \sum_{\{l,k,m\} \in M^{LK}} f_{klmt}^{sales} c_{jlm}^{transport-sales} \tag{11}$$

Storage cost in a facility is equal to the amount of material kept in inventory during each time period multiplied by its storage cost per month.

$$StorageCost = \sum_{t \in T} \sum_{\{m,l\} \in M^L} S_{mlt}^{mat} c_{lm}^{stor} \tag{12}$$

Procurement costs are equal to the flow of materials transported from each supplier to different facilities multiplied by the selling price.

$$ProcurementCost = \sum_{t \in T} \sum_{\{j,l,m\} \in M^{JL}} f_{ll'mt}^{sup} c_{lmt}^{sup} \tag{13}$$

Demand and Procurement

Suppliers and customers may offer/request materials between lower and upper fulfilment bounds, as shown in equations 14 and 15. Lower and upper bounds for customers are multiplied by binary variable θ, which is equal to one if the order is fulfilled and equal to zero otherwise. For contractual orders, the lower and upper bounds are equal, because the contractual amount is fixed. But the lower bound for spot orders is equal to zero and the model can determine what percentage of the order should be fulfilled. Equation 16 forces θ of all time periods to be equal to

θ of first time period. In this way, if an order is accepted in the first period, it must be fulfilled over all other time periods. This constrain refers to contractual orders, which either must be fulfilled throughout the year, or must be refused. This will not cause any problem for spot orders, which can be fulfilled partially at any time, because if model decides not to fulfil a spot order, model can assign zero to fulfilled amount for this order, as the lower bound for spot order fulfilment is zero, no matter if θ is zero or one. Thus, it can be said that θ is one for all spot orders and can be zero or one for contractual orders.

$$\underline{Q}_{lmt}^{supp} \leq f_{ll'mt}^{sup} \leq \overline{Q}_{lmt}^{supp} \qquad \forall \ \{j,l,m\} \in M^{LJ}, t \in T \qquad (14)$$

$$\theta_{ll'mt}^{ord}\underline{Q}_{lmt}^{sales} \leq f_{l'lmt}^{sales} \leq \theta_{ll'mt}^{ord}\overline{Q}_{lmt}^{sales} \qquad \forall \ \{l,k,m\} \in M^{LK}, t \in T \qquad (15)$$

$$\theta_{ll'm1}^{ord} = \theta_{ll'mt}^{ord} \qquad \forall \ \{l,k,m\} \in M^{LK}, t > 1 \qquad (16)$$

Transportation

A maximum transportation capacity constraint limits the amount of materials that can be transported between locations (suppliers, facilities and customers).

$$f_{jlmt}^{sup} \leq \overline{Q}_{jlm}^{transport-sup} \qquad \forall \ \{j,l,m\} \in M^{LJ}, t \in T \qquad (17)$$

$$f_{lkmt}^{mill} \leq \overline{Q}_{lkm}^{transport-sales} \qquad \forall \ \{l,k,m\} \in M^{LK}, t \in T \qquad (18)$$

Inventory Management

The material balance at a facility is equal to the previous inventory, plus/minus material coming from and going to other sites as well as the consumption/production from processes.

$$S_{mlt}^{mat} = S_{mlt-1}^{mat} + \sum_{\{j,l,m\} \in M^{JL}} f_{jlmt}^{sup} - \sum_{\{l,k,m\} \in M^{LK}} f_{lkmt}^{sales} + \sum_{\{l,l',m\} \in M^{LL}} f_{ml'lt}^{mill} - \sum_{\{l,l',m\} \in M^{LL}} f_{mll't}^{mill} - \sum_{\{l,p,m\} \in M^{P-out}} x_{lmpt}^{proc} + \sum_{\{l,p,m\} \in M^{P-in}} y_{lmpt}^{proc} \qquad \forall \{l,m\} \in M^{L}, t > 1 \qquad (19)$$

At time t=1, S_{mlt-1}^{mat} does not exist and it is replaced by the initial inventory quantity, S_{ml}^{start}.

$$S_{ml1}^{mat} = S_{ml}^{start} + \sum_{\{j,l,m\} \in M^{JL}} f_{jlm1}^{sup} - \sum_{\{l,k,m\} \in M^{LK}} f_{lkm1}^{sales} + \sum_{\{l,l',m\} \in M^{LL}} f_{ml'l1}^{mill} - \sum_{\{l,l',m\} \in M^{LL}} f_{mll'1}^{mill} - \sum_{\{l,p,m \in M^{P-out}\}} x_{lmp1}^{proc} + \sum_{\{l,p,m\} \in M^{P-in}} y_{lmp1}^{proc} \qquad \forall \{l,m\} \in M^{L}, t = 1 \qquad (20)$$

To ensure that the optimization model does not completely deplete the inventory at the end of the planning horizon ($t=T$), a constraint specifying the final minimum inventory quantity must be added.

$$S_{mlT}^{mat} \geq S_{ml}^{End} \qquad \forall \{l, m\} \in M^L, t = T \qquad (21)$$

Finally, each site has storage capacity constraints.

$$\underline{Q}_{lm}^{stor} \leq S_{lmt}^{mat} \leq \overline{Q}_{lm}^{stor} \qquad \forall \{l, m\} \in M^L, t \in T \qquad (22)$$

Recipe selection

Equations 23 to 28 constrain the selection of recipes. Each process has an offline/idle recipe that can be selected for when the process is not needed. Equation 23 demands that only one recipe (campaign) must be selected during one time period.

$$1 = \sum_{\{l,p,r\} \in R^P} \alpha_{lprt}^{rec} \quad \forall \{l, p\} \in P^L, t \in T \qquad (23)$$

Equation 24 determines the recipes that are used in the first time period.

$$\alpha_{lpr}^{start} \leq \alpha_{lpr1}^{rec} \quad \forall \{l, p, r\} \in R^P, t = 1 \qquad (24)$$

Equations 25 to 28 define binary variable β which represents the recipes that are used in at least two consecutive time periods. In the first time period β is equal to zero, as there is no time period before this period. Equations 26 to 28 make the linkage between α and β. Equations 27 and 28 ensure that β is zero, if α is zero in the same or previous time period.

$$\beta_{lprt}^{proc} = 0 \quad \forall \{l, p, r\} \in R^P, \ t = 1 \qquad (25)$$

$$\alpha_{lprt}^{rec} + \alpha_{lprt-1}^{rec} - 1 \leq \beta_{lprt}^{proc} \quad \forall \{l, p, r\} \in R^P, \ t \in T \qquad (26)$$

$$\beta_{lprt}^{proc} \leq \alpha_{lprt-1}^{rec} \quad \forall \{l, p, r\} \in R^P, \ t \in T \qquad (27)$$

$$\beta_{lprt}^{proc} \leq \alpha_{lprt}^{rec} \quad \forall \{l, p, r\} \in R^P, \ t \in T \qquad (28)$$

Production

Processes must be permanently utilized (or idled) during a time period. The available processing hours are equal to the number of hours during a time period minus scheduled maintenance shutdown and lost time during changeovers. As there is no changeover in the first time period, equation 29 only considers shutdown hours.

$$\sum_{\{l,p,r\} \in R^P} h_{lprt}^{rec} = H_{lpt}^{proc} - \varepsilon_{lpt}^{proc} \qquad \forall \{l, p\} \in P^L, \ t = 1 \qquad (29)$$

$\sum_{\{l,p,r\}\in R^P} h_{lprt}^{rec} = H_{lpt}^{proc} - \varepsilon_{lpt}^{proc} - \left(1 - \sum_{\{l,p,r\}\in R^P} \beta_{lprt}^{proc}\right) H_{lp}^{changeover} \qquad \forall\ \{l,p\} \in P^L,\ t \in T > 1$ (30)

Each recipe has minimum and maximum throughput boundaries (tons/hour).

$h_{lprt}^{rec} \underline{Q}_{lpr}^{proc} \leq y_{lprt}^{rec-tot} \leq h_{lprt}^{rec} \overline{Q}_{lpr}^{proc} \qquad \forall \{l,p,r\} \in R^P, t \in T$ (31)

Production hours are bounded between minimum campaign length and available processing hours including shutdown hours.

$\alpha_{lprt}^{rec} H_{lpr}^{camp} \leq h_{prt}^{rec} \qquad \forall\ l \in L^{mill}, p \in P_l^{mill}, r \in R_p^{proc}, t \in T$ *(32)*

$h_{lprt}^{rec} \leq \alpha_{lprt}^{rec} (H_{lpt}^{proc} - \varepsilon_{lpt}^{proc}) \qquad \forall\ l \in L^{mill}, p \in P_l^{mill}, r \in R_p^{proc}, t \in T$ (33)

Equations 34 to 36 are related to the mass balance. Equation 34 links the material conversion from feedstock to products. Linear recipe functions are used to represent process where raw material consumption depends on the utilization rate of the equipment employed. Equation 35 relates the material output to the total output of a process, while equation 36 aggregates the total output of a material during one time period.

$x_{lmpt}^{proc} = \sum_{\{l,p,r,m\}\in M^{R-in}} a_{lprm}^{input} y_{lprt}^{rec-tot} \qquad \forall \{l,p,m\} \in M^{P-in}, t \in T$ *(34)*

$y_{lprmt}^{rec} = a_{lprm}^{output} y_{lprt}^{rec-tot} \qquad \forall \{l,p,r\} \in R^P, \{l,p,r,m\} \in M^{R-out}, t \in T$ *(35)*

$y_{lmpt}^{proc} = \sum_{\{l,p,r,m\}\in M^{R-out}} y_{lprmt}^{rec} \qquad \forall \{l,p,m\} \in M^{P-out}, t \in T$ (36)

Processes require or produce steam and/or electricity for their operation. Equations 37 to 40 calculate the steam and electricity production/consumption of processes based on the recipe used.

$v_{lpt}^{output} = \sum_{\{l,p,r\}\in R^P} b_{lpr}^{output-steam} y_{lprt}^{rec-tot} \qquad \forall\ \{l,p\} \in P^L, t \in T$ (37)

$v_{lpt}^{input} = \sum_{\{l,p,r\}\in R^P} b_{lpr}^{input-steam} y_{lprt}^{rec-tot} \qquad \forall\ \{l,p\} \in P^L, t \in T$ (38)

$w_{lpt}^{output} = \sum_{\{l,p,r\}\in R^P} b_{lpr}^{output-elect} v_{lpt}^{output} \qquad \forall\ \{l,p\} \in P^L, t \in T$ (39)

$w_{lpt}^{input} = \sum_{\{l,p,r\}\in R^P} b_{lpr}^{input-elect} y_{lprt}^{rec-tot} \qquad \forall\ \{l,p\} \in P^L, t \in T$ (40)

The steam balance must be satisfied. Enough steam must be produced by boilers and other steam producing equipments to satisfy the needs of other steam consuming processes. However, extra steam may be produced and vented off if not necessary, as represented in equation 41.

$\sum_{\{l,p,r\}\in R^P} (v_{lpt}^{output} - v_{lpt}^{input}) \geq 0 \qquad \forall\ \{l,p\} \in P^L, t \in T$ (41)

5. Scenario-based approach for the strategic design of the SC network

The methodology proposed for scenario-based SC network design is shown in Fig. 3. As mentioned earlier, product/Process portfolios are defined by separate methodologies. These methodologies have been reviewed by Mansoornejad, Chambost, and Stuart (2010). The output of product portfolio definition methodology is a set of product portfolios, defined as a combination of existing P&P products and new biorefinery products that can be produced by the company. The product portfolio definition methodology feeds the techno-economic study whose goal is to, first identify the process technologies that can be used to produce the targeted products, and second define different process alternatives from identified technologies with different levels of flexibility. The result will be a set of product/process portfolios that will be used as input to our methodology. The methodology includes two parts; first, possible SC network alternatives are identified and after being combined with product/process portfolios, product/process/SC network alternatives are evaluated based on their performance at the operational level. The methodology is explained in more details in the next sections.

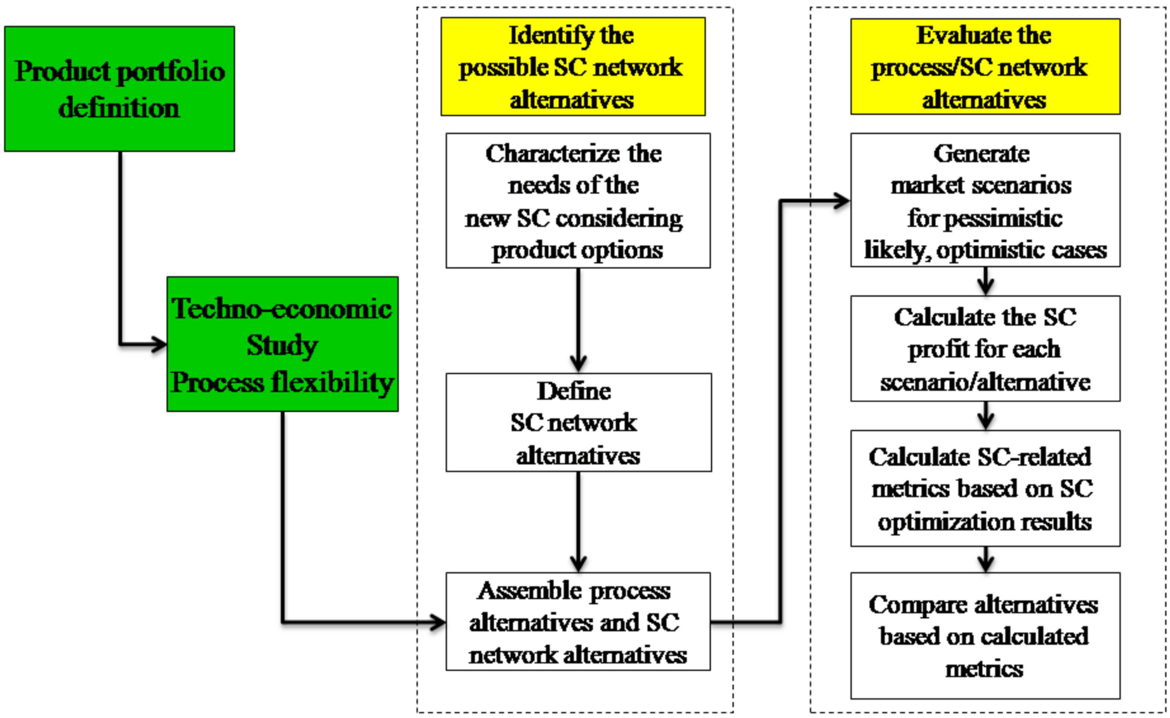

Fig. 3. Scenario-based methodology for the SC network design.

5.1. *Identify possible SC network alternatives*

5.1.1. *Identify the specifications of the new SC considering product options*

The SC networks of forest-products companies are in place with their own existing assets. Depending on the processes used in the mills, different facilities exist on the site. However, some processing steps are common among all processes in the mill, and therefore similar facilities and assets can be used or redesigned to be able to handle larger volumes.

Biomass receiving, processing, and storage areas in the mills generally include a biomass receiving and unloading station, biomass storage with a reclaimer, biomass processing involving a biomass size-reduction process, cleaning and wet storage, and finally biomass drying and dry storage. These facilities are used regardless of the fate of the biomass, i.e., the final product. Therefore, the design process should identify whether the new processes need the same facilities and whether the existing facilities have enough capacity for the larger amount of biomass that will be brought to the mill. If new or additional facilities are required, there is a need to investigate how those facilities should be modified or be added to the site to enable the mill to accept more biomass. Moreover, existing boilers, turbines, and wastewater treatment plants can be used by the new processes, which will significantly reduce the required capital cost for implementing the FBR [Janssen-suc].

On the product side, the characteristics of new products must be taken into account to redesign the SC network. Each product has specific properties and characteristics which imply specific facilities for transportation and storage. Some products can be stored in warehouses, while others must be stored in tanks. Moreover, some products are transferred by truck or train, while others should be transported in a tanker or by pipeline. Therefore, the specifications of each product must be identified so that they can be addressed when defining SC network alternatives.

5.1.2. *Define SC network alternatives*

With the existing SC assets and the characteristics of the products, the specifications of the new SC network can be identified. Based on these specifications, several SC network alternatives can be defined, which reflect the needs of the new SC network as well as the concerns of company experts. Several issues should be addressed when generating these alternatives;

- Partnership: Collaborating with other companies whose expertise brings value to the company's business model must be considered in the SC network design. Partners can cooperate in producing a product, delivering the product, buying the product, and/or selling the product to the market. In this way, a part of the partner's SC assets will be used, and less capital will be needed for establishing the new SC network.
- Location and capacity of distribution centers: based on the location of the plant, several target markets might exist in the areas around the plant. Therefore, different distribution centers with different capacities can be assigned to the target market areas. The role of partners in this issue is important. They might take the role of seller in the target markets, and they might have the required infrastructure for this purpose.
- Transportation network: Based on the characteristics of the products, different means of transportation can be used for product delivery. Again, partnerships can be used to reduce the capital costs required for establishing a transportation network. Contracts can be made with transportation companies which have a network of trucks or tankers and can simply deliver the products to markets. In addition, partners which buy the products or just deliver them to the market might have their own existing transportation network.

5.1.3. *Assemble process alternatives and SC network alternatives*

After defining the SC network alternatives, the product/process alternatives are assembled to create combined alternatives. Each combined alternative involves a process configuration with a targeted flexibility level and a SC network related to the products. The capital investment required to redesign the SC network is added to the capital investment needed for the process technologies for each alternative. The capital investment needed for the SC network alternatives which involve partnerships is smaller because a part of capital will be paid or has already been paid by the partner. However, it should be noted that the revenue will also be shared by the partner, and therefore less profit will be acquired by the company.

5.2. *Evaluate the process design/SC network alternatives*

5.2.1. *Generate price/supply/demand scenarios*

To address the uncertainty of market conditions and to reflect market volatility in the decision-making process, a scenario-based approach is used. Each scenario represents a specific market condition with respect to price, supply, and demand. Scenarios are generated in terms of feedstock supply and product demand, as well as feedstock and product prices. Scenarios must be generated to capture different market situations, that is, pessimistic, likely, and optimistic cases should be considered in scenario generation. Another important factor in scenario generation is the time aspect. Scenarios can be generated for different time scales, and depending on the type of decisions to be made in the scenario analysis, scenarios can be generated for the short, medium, or long term. For strategic design-related decisions, scenarios should be generated for the long term, e.g., for a period of several year. As supply, demand, and price change during the year, the values associated with them can vary on a monthly or seasonal basis. Note that buying feedstock and selling products can be done based either on contracts or on the spot market. Contractual prices and demands imply fixed values during specific periods, meaning that the amount of product and its price in the contract can be fixed for the whole period of the contract, while spot prices are generally subject to changes based on the market situation. Therefore, both spot and contractual prices and demands must be addressed in scenario generation.

5.2.2. *Calculate the SC profit for each scenario/alternative*

To evaluate combined alternatives, the profitability of each alternative along with other metrics must be estimated. Therefore, the SC profit associated with each alternative in different market situations must first be calculated, and then, using the profit, profitability of each alternative as well as other metrics can be estimated. In this step, the SC profit for each product/process/SC alternative is calculated for every price/supply/demand scenario. To calculate the SC profit, the SC optimization model is used. The model optimizes SC profit by determining which orders to fulfill and calculating the optimum value of production rate related to each product and the flows of material between SC nodes. The overall problem at this stage can be stated as follows. Given:

- Number and length of time intervals
- Demand and price data for each feedstock, product, market, and time interval for each scenario
- Process configuration based on what was defined in the process design alternatives
- Configuration of the SC network based on what was defined in the SC network alternatives

- Capacity data of the nodes of the SC
- Direct cost parameters, i.e., unit production, transport, handling, and inventory costs based on operating cost calculations;

With the aim of profit maximization, find

- Orders to fulfill: which contracts to make, which spot demand to fulfill
- Production rates of each product for all time intervals and all market scenarios
- Flows of materials between the plants, warehouses, distribution centers, and markets
- SC profit.

5.2.3. *Calculate SC-related metrics based on SC optimization results*

To evaluate each product/process/SC alternative, the value of several metrics should be estimated for each alternative. In this paper, SC profitability, flexibility and robustness are used as SC-related metrics.

There are several profitability estimation methods that can be used to estimate the profitability of a project. In this methodology, internal rate of return (IRR) is used as the measure of profitability. IRR is defined as the discount rate at which sum of discounted cash flows over a period becomes zero. Cash flow is calculated as the net profit minus tax. The net profit is calculated by SC optimization model.

5.2.4. *Compare alternatives based on calculated metrics*

The calculated metrics can be used to decide which alternative has better performance against market volatility and is more profitable over the long term. As mentioned earlier, the SC optimization plays the role of a tool that provides better insight into the problem. It does not aim at making the final decision and it is the human knowledge and experience that make the final decision. When having several metric/criteria, an MCDM framework can be helpful. It uses several metrics provided by different analysis tools such as SC analysis, LCA, techno-economic studies, etc., and a panel gives weights to each of those metrics based on its importance. In this way, the best alternative can be identified considering different perspectives. Fig. 4 shows the metrics provided by different analysis tools to be used in the MCDM. In this work, the MCDM is not performed and only the results coming out of the SC analysis are presented.

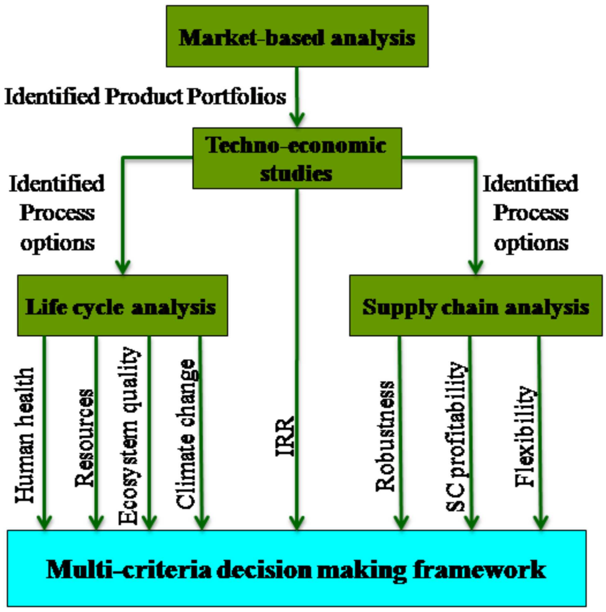

Fig. 4. MCDM framework.

6. Case study

A P&P mill aims at implementing FBR. Two product/process portfolios are considered. In the first portfolio, called Thermochemical option, Fischer-Tropsch liquids (FTL) are produced by biomass gasification and a generic gas-to-liquid process, and then are separated into waxes and diesel. Diesel can be converted into jet fuel (JF). The second portfolio, called Biochemical option, involves production of succinic acid (SA), malic acid (MA) and lactic acid (LA). All three products are produced in similar fermenters. SA and MA can be recovered in a similar recovery system, but LA needs a specific recovery system.

The process alternatives related to thermochemical option are shown in Fig. 5. All alternatives are similar up to JF production line, as shown at the top of Fig 4.a. The rest of the process is shown at the bottom of this figure for each alternative. In the first alternative, A-1, FTL is separated into waxes and diesel. The waxes are sold, and the whole diesel is converted to JF. In the second alternative, A-2, a smaller process is used to convert diesel to JF. Hence, this system would have more potential for flexibility in terms of product. The third alternative is a combination of A-1 and A-2. Two small processes are used in parallel. If both are in operation, it performs like alternative A-1 and if one of them is shut down, it performs like alternative A-2. This alternative has the highest potential for flexibility among others.

For the biochemical option, two process alternatives have been considered (Fig. 6). In the first alternative, B-1 (Fig. 6.a), there are two separate lines. The first line produces SA and MA in different production modes and the second line produces LA. In the second alternative, B-2 (Fig. 6.b), an SA/MA recovery system is added to the LA production line, so that this line can be changed over to produce SA or MA. One of SA/MA and LA recovery systems is always in standby mode. Therefore, second alternative has more potential for flexibility. It must be mentioned that all process alternatives have already been defined through studying the required level of flexibility for each portfolio. For further information, the reader is referred to Mansoornejad et al. (2012).

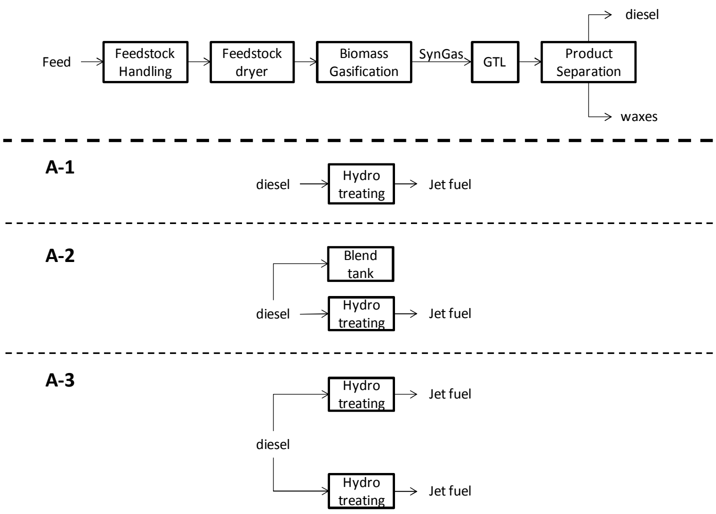

Fig. 5. Design alternatives for thermochemical option.

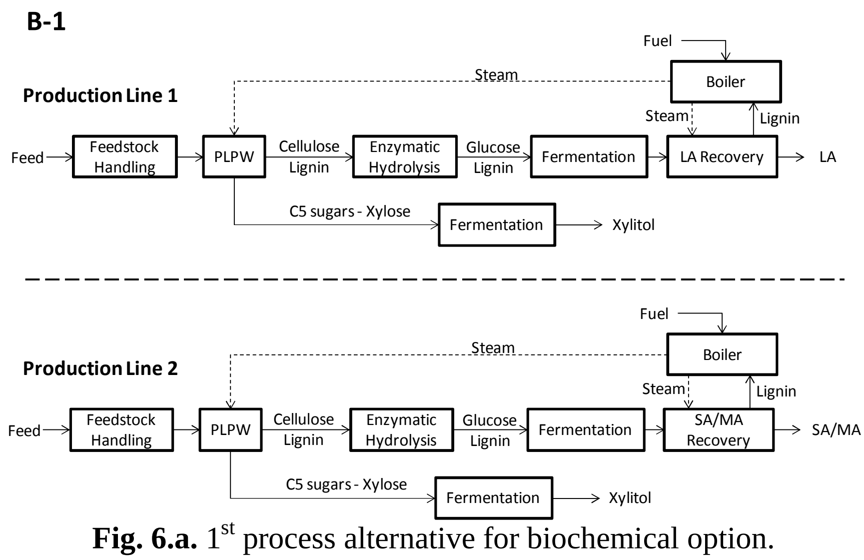

Fig. 6.a. 1st process alternative for biochemical option.

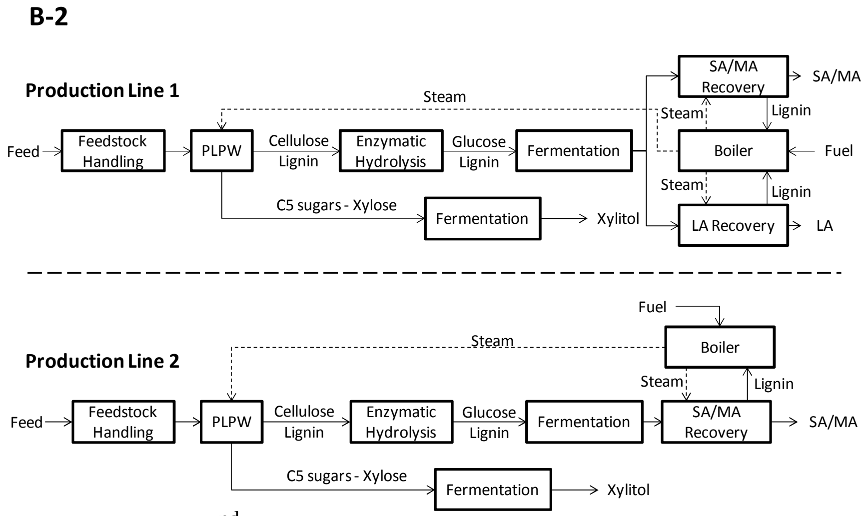

Fig. 6.b. 2nd process alternative for biochemical option.

After defining process alternatives, SC network alternatives must be defined and combined with the process alternatives. The new products are characterized and based on them, type of storage and transportation systems for each of them are identified. More importantly, partnership strategies for each alternative are defined. Table 1 and Table 2 show the SC network alternatives defined for the each portfolio option. Company's restrictions and policies must be considered in the definition of the SC network alternatives. Therefore, different processing, selling strategies, transportation and partnership shown in these tables are defined by the mill's executives. Thermochemical option, which has three process alternatives, has six SC network alternatives. Each process alternative is associated with two SC network alternatives. Biochemical option has two process alternatives. Two SC network alternatives are associated with each of them, making four SC network alternatives in total.

The SC networks are defined considering the process options. For process alternative A-1, which can potentially convert the whole diesel into JF, there are two SC network alternatives at the processing stage; either making partnership with a JF producer which in turn implies a specific selling strategy for diesel, i.e. selling diesel completely to JF producer, or producing JF at the mill. For process alternative A-2, which can produce both diesel and JF, there are two SC networks alternatives at the sales level for diesel; either making a contract with a partner and sending diesel to him, or selling it on the spot. For process alternative A-3, there are two SC network alternatives at the transportation level for wax and diesel; either buying trucks, or making contract with a transportation company.

For process alternative B-1 and B-2, SC network alternatives are different at processing level. There are two alternatives; either sending the extractives (hemicelluloses and C5 sugars) to a partner for more processing, or processing them at the mill. Moreover, different transportation strategies can be defined.

Table 1 SC network alternatives defined for portfolio 1

	A-1	**A-2**	**A-3**
Processing	Partnership with JF producer OR Producing JF at the mill	Producing JF at the mill	Producing JF at the mill
Selling	Waxes: Contract & Spot Diesel: - To JF producer OR -To be converted to JF Jet fuel: Contract	Waxes: Contract & Spot Diesel: - Contract with a partner OR -Spot Jet fuel: Contract	Waxes: Contract & Spot Diesel: Contract & Spot Jet fuel: Contract & Spot
Warehousing	Expansion	Expansion	Expansion
Delivery/ Transportation	Wax delivery - Buy trucks Partnership for JF delivery	Wax and diesel delivery -Buy trucks Partnership for JF delivery	Wax and diesel delivery -Buy trucks OR -Contract with a partner Partnership for JF delivery

Table 2 SC network alternatives defined for portfolio 2

	B-1	**B-2**
Processing	Send extractives to partner OR Process extractives at the mill	Send extractives to partner OR Process extractives at the mill
Selling	SA: Contract & Spot MA: Contract & Spot LA: Contract & Spot	SA: New market for Contract & Spot MA: Contract & Spot LA: Contract & Spot
Warehousing	Expansion	Expansion
Delivery/ Transportation	Buy trucks OR Contract with a logistics partner	Partnership for SA delivery/selling -Buy trucks OR -Contract with a logistics partner

The total capital investment required for each combined alternative is shown in Table 3.

Table 3 Capital investment of combined alternatives

Portfolio 1			**Portfolio 2**		
Process alternative	SC network alternative	Capital ($MM)	Design alternative	SC network alternative	Capital($MM)
A-1	Partner for JF	61	B-1	Sell extractives	113
	Produce JF	87		Process extractives	122
A-2	Diesel on spot	78	B-2	Sell extractives	122
	Partner for diesel	76		Process extractives	131
A-3	Own fleeting	98			
	Partnership	95			

Market scenarios for each option, representing market volatility, are presented in Fig. 7 and Fig. 8.

Fig. 7. Market scenarios for the Thermochemical option

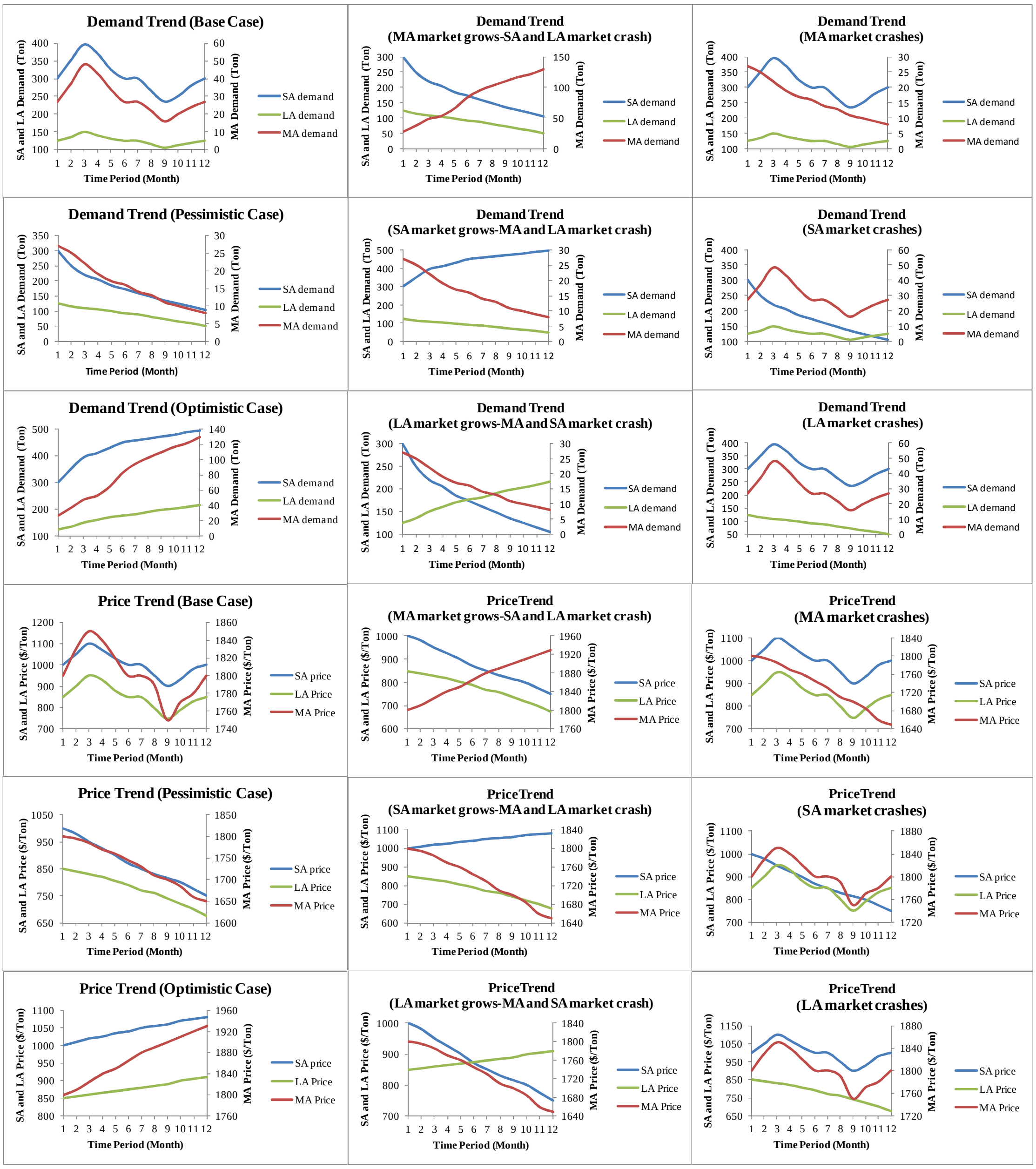

Fig. 8. Market scenarios for the Biochemical option

Base-case profitability, flexibility and robustness of process alternatives (combined alternatives excluding SC network alternatives) are depicted in Fig. 9. The value of flexibility metric shown in this graph is the average flexibility used by each alternative in all scenarios. As shown by the flexibility metric in this figure, as the potential for flexibility increases, more flexibility is used. Moreover, as more flexibility is used, robustness increases, meaning that the SC is more robust against volatility. But profitability does not have the same behaviour as flexibility increases. It is illustrated that alternative A-3, which has the highest potential for flexibility and also more flexibility is used on this alternative, has the lowest profitability. That is due to the fact that profit improvement as a result of higher flexibility cannot compensate the increase in capital cost and the extra capital cost paid for more flexibility is not paid off in this case. The profit acquired by each combined alternative for thermochemical option is presented in Fig. 10. It can be seen that the profits of all alternatives in each market condition are close to each other, though the alternative A-3 with own fleeting has the highest profit.

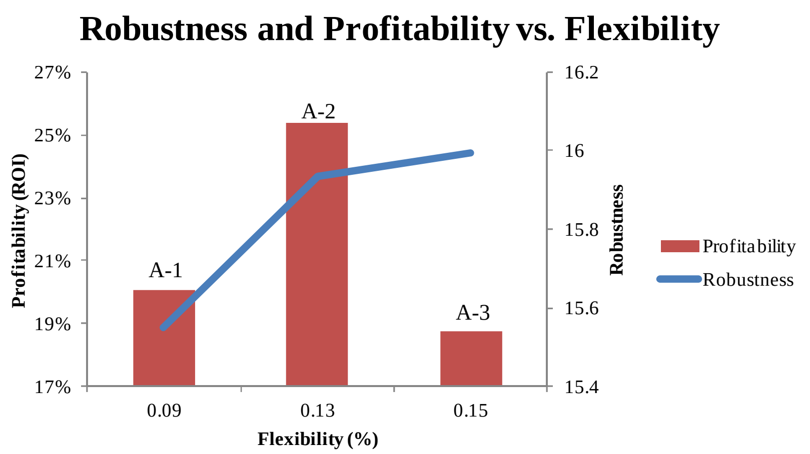

Fig. 9. Robustness and profitability vs. flexibility: Thermochemical option

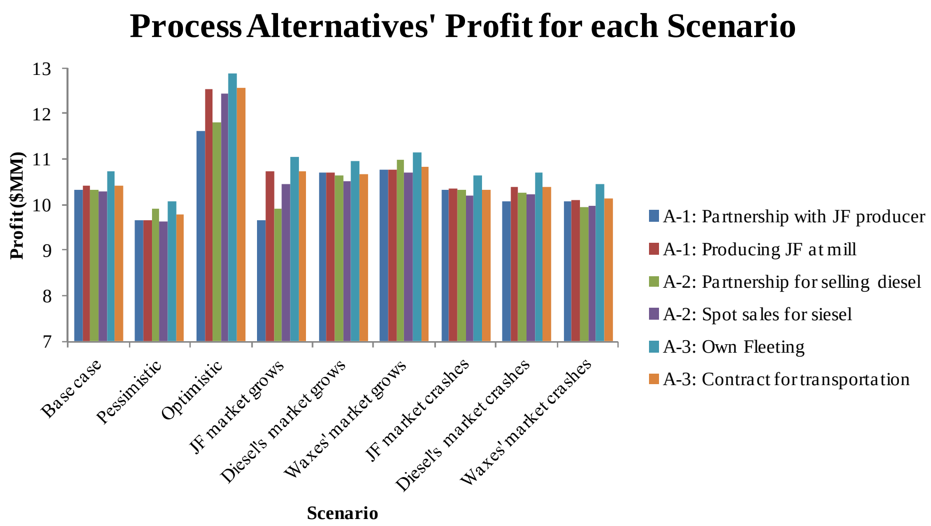

Fig. 10. Profit of combined alternatives for all scenarios: Thermochemical option

The results for each combined alternative are presented in this section. Process alternative A-1 has two SC network alternatives at the processing level, one implying sending diesel to a JF producer and one including JF production at the mill. The IRR and robustness of these two combined alternatives are illustrated in Fig. 11. The IRR of the option of sending diesel to JF producer is much higher than that of producing JF at the mill. It means that producing JF at the mill, with current price or production cost, is not profitable. Therefore, company may sell its diesel to a JF producer which will also secure company's diesel market. But, it can be seen that the robustness of the option of producing JF at the mill is higher. That is because of the increase in flexibility. The system is more flexible when it produces one more product. It gives more flexibility to the company in a volatile market, and thus makes it more robust against market volatility.

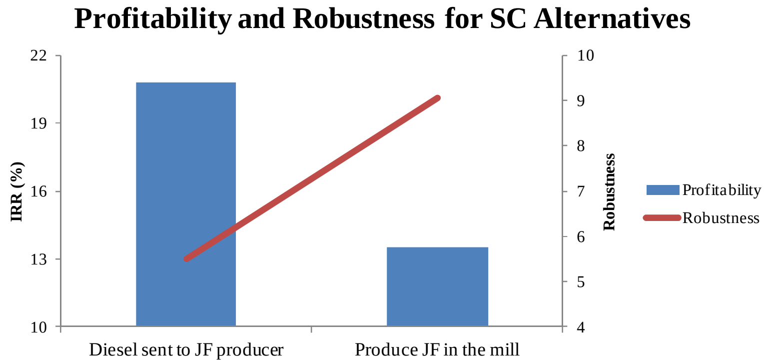

Fig. 11. Profitability and Robustness for SC Alternatives: A-1

Process alternative A-2 has two SC network alternatives at the sales level; sending diesel to a partner or selling it on the spot. Figure 3-35 reveals that both alternatives have almost equal IRR, but robustness of sending diesel to a partner is higher. The reason is that in this way the company externalizes the risk of facing with volatility in diesel market by transferring it to the partner.

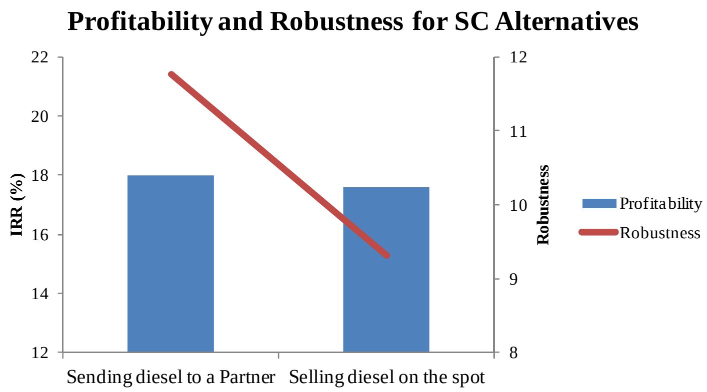

Fig. 12. Profitability and Robustness for SC Alternatives: A-2

Process alternative A-3 is associated with two SC network alternatives at the transportation level; buying trucks, i.e. own fleeting, or making contract with a transportation company. Fig. 13

shows that both alternatives have almost equal IRR and robustness. Thus, although from an economic point of view there is no difference between these two alternatives, second alternative implies less risk and responsibility. Instead of buying a network of trucks and taking care of them and their logistics, the company can easily outsource its transportation system and still have the same economic result.

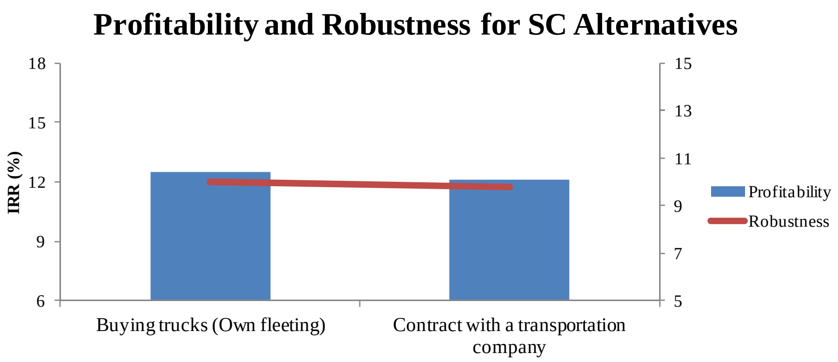

Fig. 13. Profitability and Robustness for SC Alternatives: A-3

Same results are presented in Fig. 14 and Fig. 15 for the Biochemical option. It is clear that by increasing flexibility in this option, the profit is improved considerably. Fig. 14 reveals that by increasing the potential for flexibility, more flexibility is used. Moreover, with more flexibility, profit (Fig. 15) and robustness (Fig. 14) are enhanced. Contrary to Thermochemical option, profitability also improves as flexibility increases. This means that for the Biochemical option, the extra capital cost paid for adding one recovery system for SA/MA to the first production line is very well compensated by the increase in capability of system to produce more profitable products.

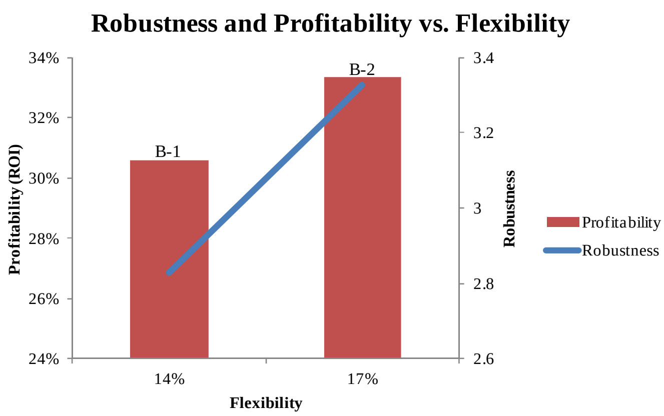

Fig. 14. Robustness and profitability vs. flexibility: Biochemical option

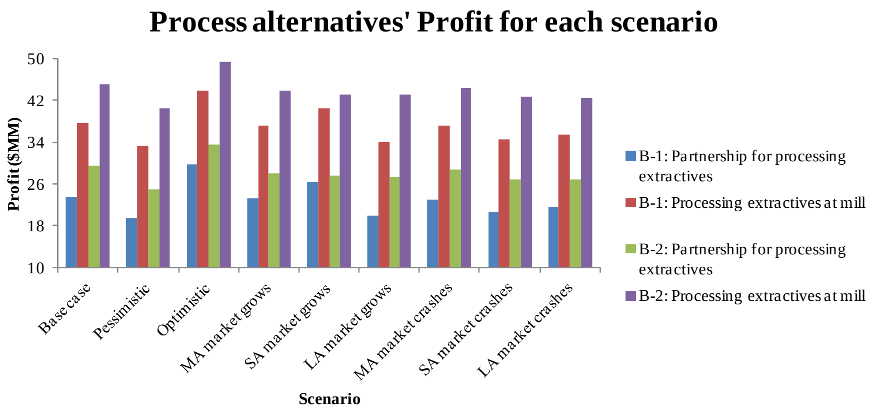

Fig. 15. Profit of combined alternatives for all scenarios: Biochemical option

The process alternatives of Biochemical option have two SC network alternatives at the processing level; either sending the extractives to a partner or processing them at the mill. Unlike the Thermochemical option for which producing JF at the mill is less profitable than sending it to a JF producer, for the Biochemical option processing the extractives at mill is much more profitable than sending it to a partner, as illustrated in Fig. 16. This is due to the fact that extractives being processed at the mill are used to produce xylitol, which is a very high value product. The results approve that added-value products can significantly increase the profitability of a company compared to commodities. The high profit associated with added-value chemicals helps them internalize the risk of volatility, i.e. the profit may decrease due to market volatility, but remains still high compared to commodities. In addition, robustness of the alternatives which involve processing the extractives at the mill is considerably higher than the robustness of alternatives which include sending the extractives to a partner. This again supports the notion that robustness improves with flexibility. The flexibility of the system is higher in the case the extractives are processed at the mill, because of producing one more product.

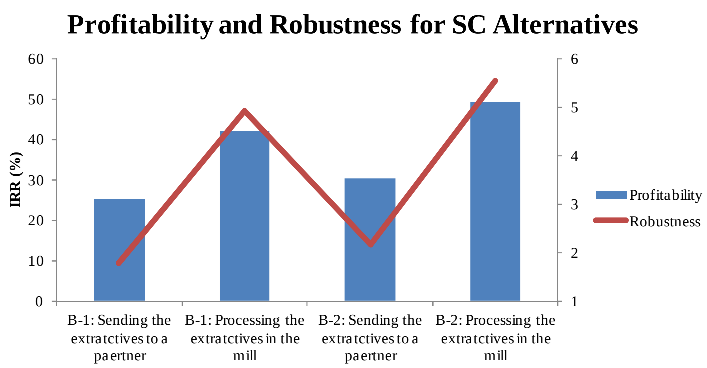

Fig. 16. Profitability and Robustness for SC Alternatives: Biochemical option

An important point to be mentioned is that the design of a process alternative affects the design of SC network alternatives and the strategies of SC management at the operational level. Fig. 17 and Fig. 18 illustrate that, in similar market conditions, different patterns of order acceptance is chosen for different levels of flexibility, i.e. for option B-1 and option B-2, which might imply different inventory management, different sales strategies, and different transportation strategies.

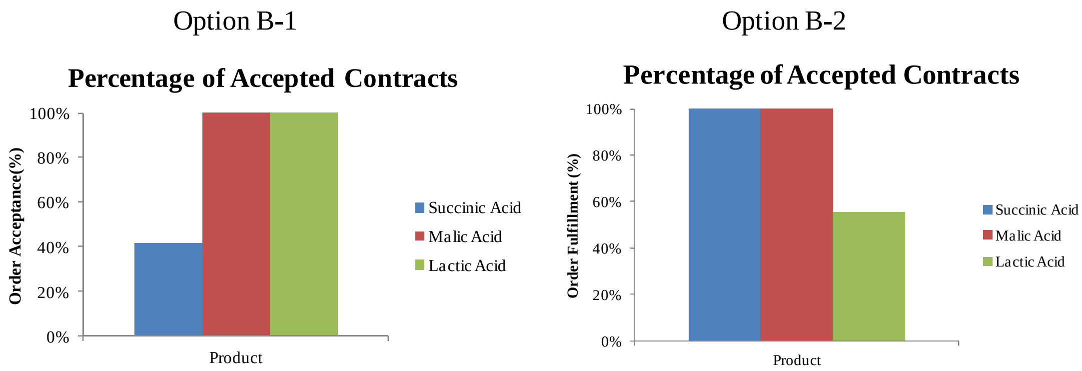

Fig. 17. Percentage of accepted contracts: Biochemical options

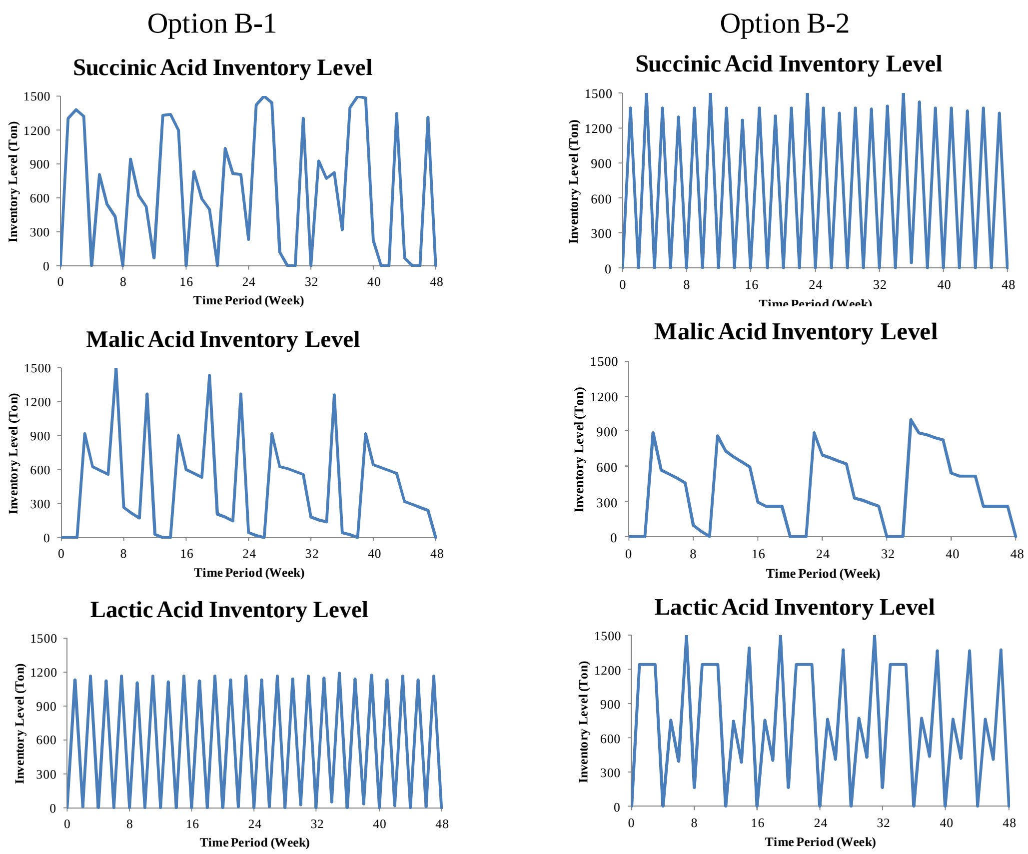

Fig. 18. Inventory levels: Biochemical options

It is shown that when the flexibility of the processes is increased, the production capacity of processes changes. In this case, some new opportunities might be found for the company in the market. That will change the strategies of the company, because the new opportunity may imply a specific partnership, sales strategy, new warehouses or new transportation system or transportation strategy. Moreover, a specific level of flexibility requires a specific inventory limit and transportation capacity. These are SC network design issues that are linked to and affected by the process considerations. This implies that designing the SC network consistent with process flexibility is very important. There is a direct relationship between level of flexibility and the configuration and specifications of the SC network, and thus, it is worth integrating them.

In conclusion, it can be said that the biochemical option is much more profitable than the thermochemical option. The potential for flexibility in the biochemical option is used better compared to the thermochemical option and thus it is more robust against market volatility. For the thermochemical option, partnership in all levels makes the project more profitable, while for the biochemical option, partnership at the processing level reduces the profitability of the project. Other factors in this regard come to the table such as access to enough capital for implementing the project. Partnership in other levels such as transportation and sales might make the project more profitable. The defined product portfolio option must be analyzed by other tools, e.g. LCA, so that other aspects of implementing such projects are revealed. Ultimately, an MCDM framework can takes into account all different aspects for making the final decision.

7. Conclusions

In the real world, forestry companies face limited options in terms of future strategies, product/process options, access to biomass, product market, etc. These all limit the choice of a company for its future. Therefore, instead of using large-scale SC mathematical formulations which consider thousands of options, a practical scenario-based approach can be used to identify the possible options and evaluate their performance in the long run. Biorefinery options involving product portfolio, process alternatives and SC network configurations considered by a company willing to implement the biorefinery, can be evaluated using the scenario-based methodology proposed in this paper. By comparing the profitability of alternatives as well as their robustness in volatile market conditions, and by screening out the non-profitable ones, a set of biorefinery options to be considered can be identified.

Furthermore, it was shown by the results that a specific level of flexibility affects the strategies in sales, partnership and transportation. With the proposed approach, i.e. defining SC alternatives related to process alternatives, the following aspects can be addressed relative to process alternatives:

- As a result of change in level of flexibility and thus, change in production capacity, the procurement, transportation, and selling costs and strategies will be different. Only a SC analysis can takes into account all these changes.
- The inventory levels and storage capacity will also be different for different levels of flexibility. Again, a SC analysis can calculate the inventory level of each product according to the production scheme and determine the storage capacity required for each product.

Acknowledgements

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APPENDIX E - Article: A systematic biorefinery supply chain design methodology incorporating a value-chain perspective

A systematic biorefinery supply chain design methodology incorporating a value-chain perspective

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The forestry industry business environment in North-America and Europe is changing. Decreasing product demand and increased competition for feedstock and market share are driving companies to seek alternative business models to be competitive over the longer term. One alternative is to enter the bio-energy and biorefinery sectors that have been emerging in recent years. The forest biorefinery (FBR) is emerging as a new possibility for improving forestry companies' business models, however introduces significant technological, economic and financial challenges. Many different strategies can be pursued for implementing the biorefinery. Due to a lack of capital for implementing such strategies, technological risks and product market immaturities, the implementation should be executed in a phase-wise manner. Proper analysis tools are required to identify feasible strategies and their implementation phases.

Design and management of supply chain (SC) is critical for the long-term competitive advantage of companies who would like to implement the biorefinery. In this regard, SC analysis can play a key role in evaluating the potential SC performance of different biorefinery implementation strategies. An SC analysis calculates the profit across the entire SC and accounts for cost contributors that are typically ignored in economic analyses, e.g. inventory cost, changeover cost, etc. It can also be used to take into consideration market volatility, and to determine how the flexibility of the manufacturing system can be exploited to mitigate market risks in order to maximize profit. In this way, SC analysis can be used to target the desired level of flexibility of a manufacturing system needed to mitigate the impact of market price volatility. Moreover, these capabilities provide better insight into the costs and profit incurred by an implemented strategy [1]. Thus, an SC analysis can be used for two different purposes:

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- For making design decisions, and more specifically, for targeting the level of flexibility of a system and designing the SC network configuration
- For comparing several strategies by evaluating their performance for different market conditions

The objective of this paper is to illustrate a hierarchical design methodology for targeting the required level of flexibility, designing the SC network configuration, and evaluating different FBR strategies for transforming a forestry company. More specifically, the aspects that will be addressed by the hierarchical methodology presented in this work include:

1. Targeting the design of flexibility, including the determination of the production capacity as well as the operating window as a design target, i.e., range of production rates for each process, showing the flexibility capability of the plant.
2. SC network design, including determination of the number of facilities of each type, the location of each facility, and the capacity of warehouses and distribution centers, as well as partner selection.
3. Evaluating the phased implementation approach, including the analysis of the implementation strategies for each biorefinery option and comparing the results.

The methodology uses an SC mathematical formulation that calculates the SC profit of each product/process option for different market scenarios. The SC formulation is also used to calculate three metrics; SC profitability, a metric of flexibility and a metric of robustness. These metrics are used for evaluating and comparing the performance of strategies.

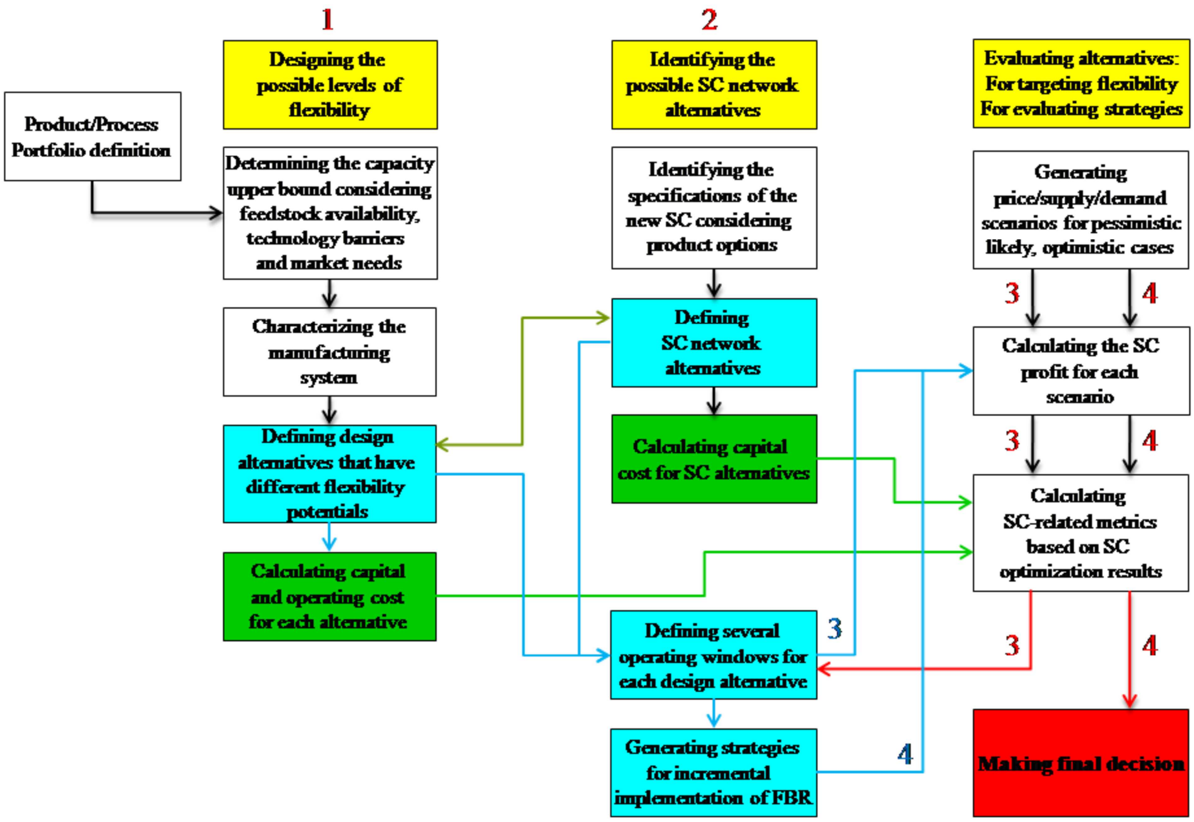

Figure 1. Hierarchical methodology for SC strategic design

Hierarchical methodology for SC strategic design

The hierarchical methodology consists of four main parts:

1. Process design: Designing possible levels of flexibility (process alternatives)
2. SC network design: Designing possible SC networks (SC network alternatives)
3. Targeting the level of flexibility for each alternative using SC optimization
4. Generating implementation strategies based on defined process/SC network alternatives and evaluating them for making the final decision

In this methodology, first, process design alternatives representing different potentials of flexibility are defined. This part includes determining the upper bound for production capacity, characterizing the manufacturing system in terms of product and volume flexibility to identify the modifications needed for the processes to become more flexible, generating design alternatives with different flexibility potentials, and calculating capital and operating cost for each design alternative. In the second part, SC network alternatives are defined based on the assets of the existing SC and resources that are needed for new products. This step involves identifying the specifications of the new SC based on the characteristics of the new product options, and defining SC network alternatives. Then the process and the SC network alternatives are combined to create a set of process-SC network alternatives, called combined alternatives. In the third part, the level of flexibility is targeted. This part contains three steps: after defining several volume flexibility levels (operating windows) for each design alternative, first, a finite number of market scenarios are generated. Then, for all flexibility levels, the SC profit is calculated for each scenario. SC model is run for different levels of volume flexibility of each combined alternative, in case of several market scenarios and SC profit of each combined alternative is calculated at the operational level over a year. Using profit and capital costs, profitability of each alternative is estimated. Moreover, the flexibility and robustness of each alternative against all market scenarios is determined using relevant metrics. These metrics, i.e. profitability, robustness and flexibility, are used to evaluate the performance of alternatives and the level of flexibility of the alternative that has the best performance is targeted as the target level of flexibility. In the fourth part, several implementation strategies are defined based on the targeted level of flexibility. The policies of the company as well as the advantages and constraints of the mill must be considered in defining strategies through discussion with mill executive. The SC model is run again for each strategy in case several market scenarios and the performance of each strategy at the operational level is evaluated using the same metrics.

SC mathematical formulation

The SC framework is formulated as an optimization problem which maximizes profit by selecting profitable orders and by calculating the optimal value of production volume, amount of required feedstock, feedstock and product inventory level, and amount of feedstock and product to be transported. This framework is an operational model which considers the management of a multi-product, multi-echelon SC, including existing production and warehousing facilities as well as a number of customer zones, although it can also be used for design purposes. Different types of biomass are provided by several suppliers. Production facilities can make one or several products. Processes are either dedicated, i.e. they produce only one product, or flexible from a product perspective, i.e. they are able to produce several products using different recipes (production modes). In other words, a flexible process can use different recipes to produce different products. Changing from one recipe to another incurs changeover cost and time.

Processes can be idled or shutdown for scheduled maintenance. The steam required for each process is provided by both fuel and biomass. Warehouses can receive material, either feedstock or product, from different sources and plants, and supply different markets. Each market places demand in two ways: by contract, i.e., for the long term, and in the spot market, i.e., for the short term. In case of a contract, specific quantities of products must be sold to the customer in specific time periods. The spot demand can be partially fulfilled. Transportation routes link suppliers, facilities and customers together. The model is formulated as an MILP problem with a discrete time horizon of 48 weeks. It is run for every week over a year. Each time period is broken down into hours. Several subsets have been created to link parameters and variables to each other, e.g. some customers accept products from specific mills and processes can produce certain materials. SC formulation is inspired by the model presented by Kannegiesser (2008) [2].

Metrics for evaluating the biorefinery supply chain performance

There are three metrics used in the methodology to evaluate the performance of designed SC in different market conditions; SC profitability, robustness and flexibility. These metrics are directly employed for decision making in this work.

Generally in economic analyses, the profitability measures consider the costs incurred by the process. Some SC-related costs such as procurement cost and transportation cost are taken into account in profitability calculations, but some other costs, which are related to the dynamism and volatility of the production environment such as inventory cost and changeover cost, are typically ignored. The internal rate of return (IRR) used in this study as a SC profitability metric considers all cost contributors over the long term to provide a better cost representation at the decision-making level.

In a robust design the control parameters of a system are selected in such a way that the desirable measured function do not diverge significantly from a given value [3]. A simple metric of robustness (MF) is used to quantify the robustness of design options against market volatility so that design options can be compared in terms of robustness, as shown in equation 1.

$$\mathrm{MR} = \left(\frac{\sum_{\mathrm{Sc}}(\mathrm{Pr_B} - \mathrm{Pr_{Sc}})}{\mathrm{Pr_B}}\right)^{-1} \qquad (1)$$

where $\mathrm{Pr_B}$ is the base case profit, $\mathrm{Pr_{Sc}}$ is the profit for scenario Sc and $\mathrm{N_{Sc}}$ is the number of scenarios. In this work, the desired parameter that must not diverge from a given value is profit.

It is desirable that the profit of a design option in case of each market scenario does not deviate from the base case profit, if this profit is lower than the base case profit. Therefore, to quantify the downside risk of volatility, calculated profits that are less than the base case profit are considered in this equation. The MR shows the percentage of aggregate deviation from the base case profit for all profits that are less than the base case profit. The smaller this percentage is the better and more robust the system will be. Hence, the reverse of the percentage is used, so that the higher values of MR represent more robust systems.

The concept of manufacturing flexibility in the FBR implies the ability to produce several bioproducts (product flexibility) at different volumes (volume flexibility) and in different time periods based on product price and demand. In the design of chemical processes, volume flexibility has a critical role. Thus, in order to design or analyse the flexibility of a system, quantifying volume flexibility is of crucial importance. Inspired by the work of Voudouris (1996) on qualitative measure of flexibility [4], metric of flexibility (MF) quantifies volume flexibility, as shown in equation 2:

$$\mathrm{MF} = \sum_{t}\sum_{p}\sum_{m}\left|\frac{C_{mpt}-C_{mp}^{N}}{C_{mp}^{N}}\right| \qquad (2)$$

where C_{mpt} is the amount of product m that is produced on process p in time period t and C_{mp}^{N} is the amount of product m produced on process p by the nominal production rate over the same number of processing hours. This formulation shows the deviation from the nominal production rate in a dimensionless form and implies volume flexibility.

Case example

A P&P mill aims at implementing FBR by producing organic acids. The product portfolio involves production of succinic acid (SA), malic acid (MA) and lactic acid (LA). All three products are produced in similar fermenters. SA and MA can be recovered in a similar recovery system, but LA needs a specific recovery system. The block flow diagram of the Biochemical option is shown in Figure 2. First line operates in one production mode and produces LA. Second line operates in two distinct production modes, producing SA in one production mode and MA in the other production mode.

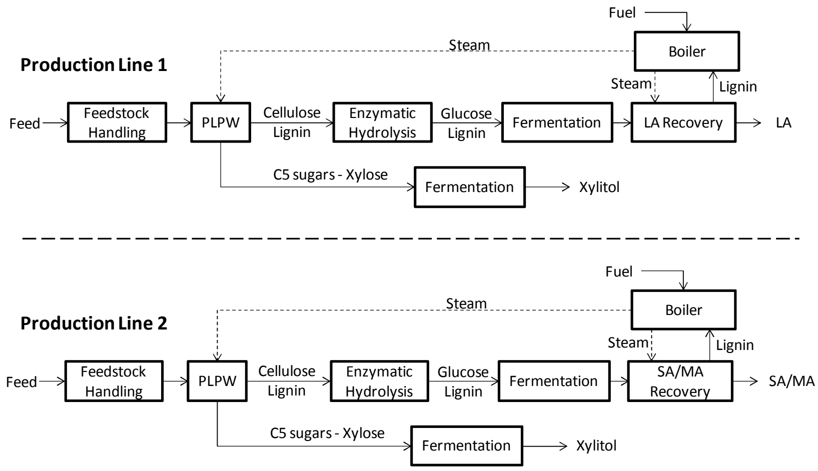

Figure 2. Process block flow diagram

Based on a market assessment, the executive board of the mill targets an acid production system requiring 1000 bone-dry tons per day of woody biomass. The characterization of system is presented in Table 1. This characterization helps to define design alternatives representing different flexibility potentials. Process alternatives representing different flexibility potentials are illustrated in Figure 3.

Table 1. Process characteristics for each option

Portfolio option	Characteristics
Biochemical Lactic acid, Succinic acid, Malic **acid**	Type of process: Semi-continuous (Batches in series) Process configuration: Lines in parallel Product flexibility: All products can be produced in similar fermenters, but in different modes. They need specific recovery systems Volume flexibility: Each process has 5% volume flexibility

Two process alternatives have been considered, as shown in Figure 3. In the first alternative, B-1, there are two separate lines. The first line produces LA and the second line produces SA and MA in different production modes. As mentioned before, all processing steps up to the recovery systems are similar in both lines. Thus, in the second alternative, an SA/MA recovery system, shown in red in Figure 5, is added to the LA production line, so that this line can be changed over to produce SA or MA as well. One of SA/MA and LA recovery systems is always in standby mode. Hence, second alternative has more potential for flexibility.

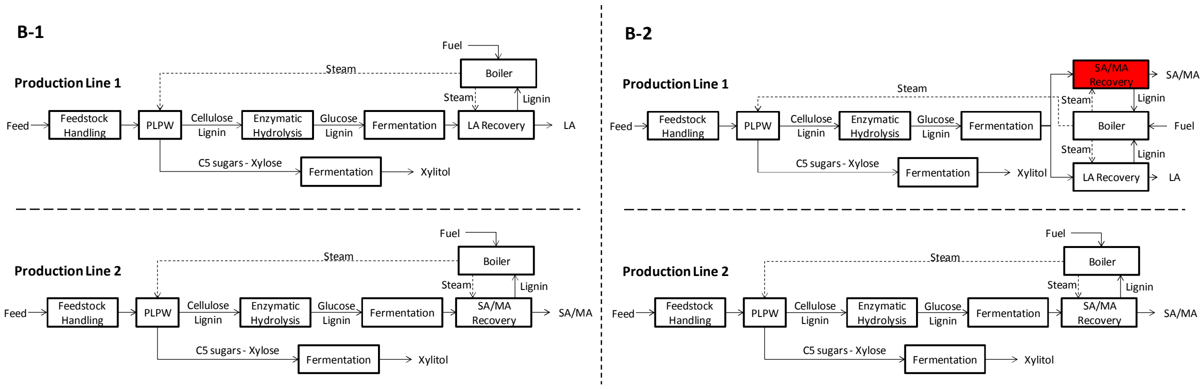

Figure 3. Process alternatives: Biochemical option

After defining process alternatives, SC network alternatives must be defined and combined with the process alternatives. Table 2 and Table 3 show the SC network alternatives defined for the each portfolio option. Company's restrictions and policies must be considered in the definition of the SC network alternatives. Different processing, selling strategies, transportation and partnership shown in these tables are defined by the mill's executive board.

Table 2. SC network alternatives

	B-1	B-2
Processing	Send extractives to partner OR Process extractives at the mill	Send extractives to partner OR Process extractives at the mill
Selling	SA: Contract & Spot MA: Contract & Spot LA: Contract & Spot	SA: New market for Contract & Spot MA: Contract & Spot LA: Contract & Spot
Warehousing	Expansion	Expansion
Delivery/ Transportation	Buy trucks OR Contract with a logistics partner	Partnership for SA delivery/selling Buy trucks OR Contract with a logistics partner

The total capital investment required for each combined alternative is shown in Table 3.

Table 3. Capital investment of combined alternatives

Design alternative	SC network alternative	Capital($MM)
B-1	Sell extractives	113
	Process extractives	122
B-2	Sell extractives	122
	Process extractives	131

SC optimization model is run for different operating windows (different levels of flexibility) of each alternative in case of several market scenarios presented in Table 4.

Table 4. Market scenarios for the Biochemical option

Scenario	Definition	Justification
Sc.1: Base case	Sinusoidal trend for price and demand of all products	Showing the volatility in the price and demand of products
Sc.2: Pessimistic	Price and demand of all products decline	Testing system's response in a situation in which market is weak
Sc.3: Optimistic	Price and demand of all products increase	Testing system's response in a situation in which market is strong
Sc.4	MA market grows, SA and LA market crash	Testing system's response in a situation when MA market is stronger than SA and LA markets
Sc.5	SA market grows, MA and LA market crash	Testing system's response in a situation when SA market is stronger than MA and LA markets
Sc.6	LA market grows, MA and SA market crash	Testing system's response in a situation when LA market is stronger than MA and SA markets
Sc.7	MA market crashes, SA and LA market follow the base-case trend	Testing system's response in a situation when MA market is weaker than SA and LA markets
Sc.8	SA market crashes, MA and LA market follow the base-case trend	Testing system's response in a situation when SA market is weaker than MA and LA markets
Sc.9	LA market crashes, SA and MA market follow the base-case trend	Testing system's response in a situation when LA market is weaker than SA and MA markets

The result of this step is shown for alternative B-1 in Figure 4, Figure 5 and Figure 6. As can be observed in Figure 4, profit improves with increasing flexibility up to 30%. Above 30%, the profit is not improved due to market conditions.

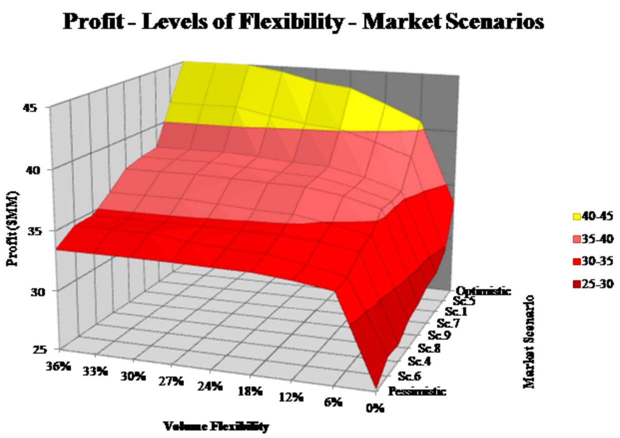

Figure 4. SC profit of each level of flexibility in case of market scenario realizations: B-1

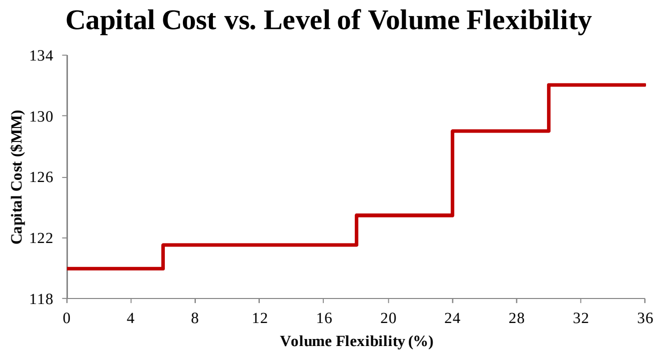

Figure 5. Capital cost for different levels of volume flexibility: B-1

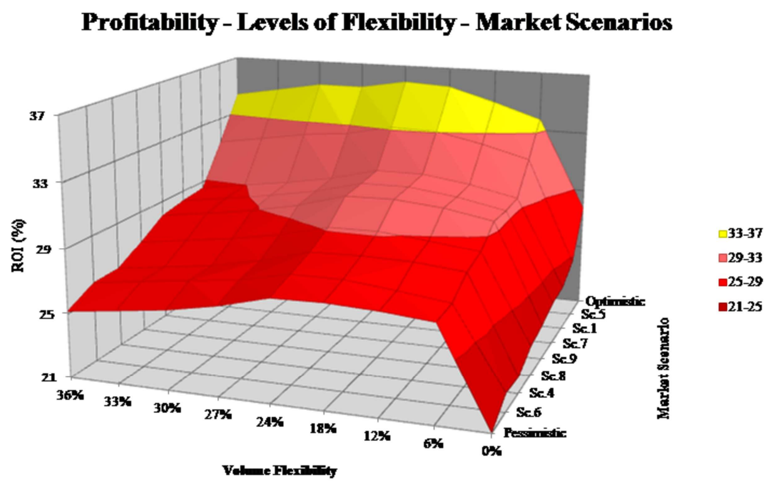

Figure 6. SC ROI of each level of flexibility in case of market scenario realizations: B-1

Figure 5 illustrates the capital cost required for each flexibility level. From 0% to 24% volume flexibility, the increase in the capital cost is not significant, because with some slight modifications the level of flexibility can be improved. In order to go beyond this level, major modifications are required to be done on the process, which incur more cost. The result of profitability (ROI) analysis is shown in Figure 6. Up to 24% flexibility, the increase in capital cost can be compensated by the profit improvements. In flexibility levels higher than 24%, the capital cost rise plays the major role and profit improvement in this range is not enough to pay off the extra capital cost. Hence, 24% can be targeted as the optimum level of flexibility for this alternative.

Process alternatives have two SC network alternatives at the processing level; either sending the extractives to a partner or processing them at the mill. As illustrated in Figure 7, processing the extractives at mill is much more profitable than sending it to a partner in both process alternatives. This is due to the fact that extractives being processed at the mill are used to produce xylitol, which is a very high value product. The results approve that added-value products can significantly increase the profitability of a company. The high profit associated with added-value chemicals helps companies internalize the risk of volatility, i.e. the profit may decrease due to market volatility, but remains still high compared to commodities. In addition, robustness of the alternatives which involve processing the extractives at the mill is considerably higher than the robustness of alternatives which include sending the extractives to a partner. This supports the notion that robustness improves with flexibility. The flexibility of the system is higher in the case the extractives are processed at the mill, because producing one more product gives more flexibility to the system in a volatile market.

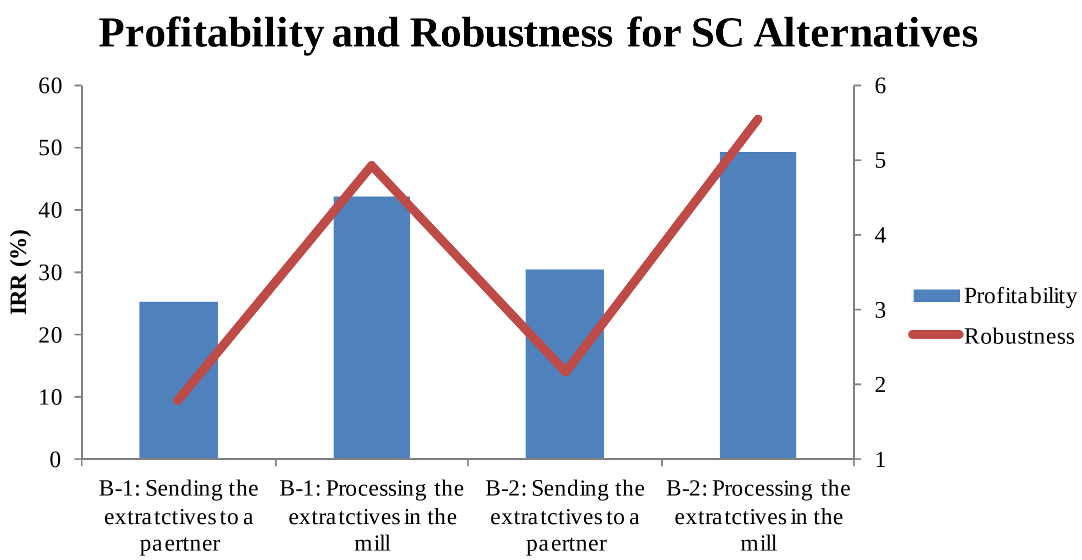

Figure 7. Profitability and Robustness for SC Alternatives

In the final step, three strategies are defined. Each strategy is implemented through one or more than one phases. These strategies are introduced in Figure 8. Strategy I consists of one phase in which one line for producing LA is installed. Strategy II comprises of two phases; in the first phase LA production line is installed and in the second phase, the second line for producing SA and MA is added. Strategy III is done within three phase; in the first phase LA line is installed, then second line will be added to produce SA and MA, and finally an extra recovery system for SA and MA will be added to the first line to make it capable of producing all three acids.

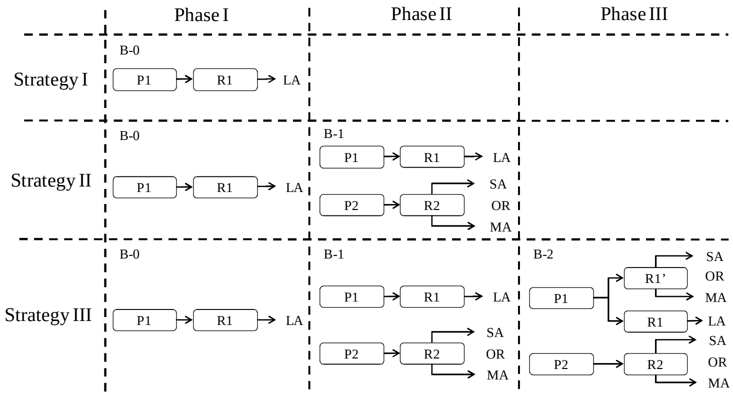

Figure 8. Phased implementation strategies: Biochemical option

The assumptions for the profitability analysis are summarized in Table 5.

Table 5. Assumption for profitability analysis

Item	Description
Depreciation	Linear over 20 years
Tax	10%
Project start date	2013 45% of total capital spending
Duration of construction	2 years
Capital cost expenditure	50% each year
Phase II implementation	In the 5th year after start-up (taking 2 years) 47% of total capital spending
Phase III implementation	In the 9th year after start-up (taking 1 year) 8% of total capital spending
Price change	2% every year

The result of profitability analysis for nine major market scenarios is presented in Figure 9. The IRR of strategy II and strategy III are much higher than that of strategy I. It implies that producing more value-added products such as SA and MA improves the profitability of the strategies. The IRR of Strategy III is also higher than that of strategy II in all scenarios, which denotes that increasing flexibility will have a positive effect on the profitability and the extra capital cost will be compensated. Figure 10 affirms that both profitability and robustness improve by increasing flexibility.

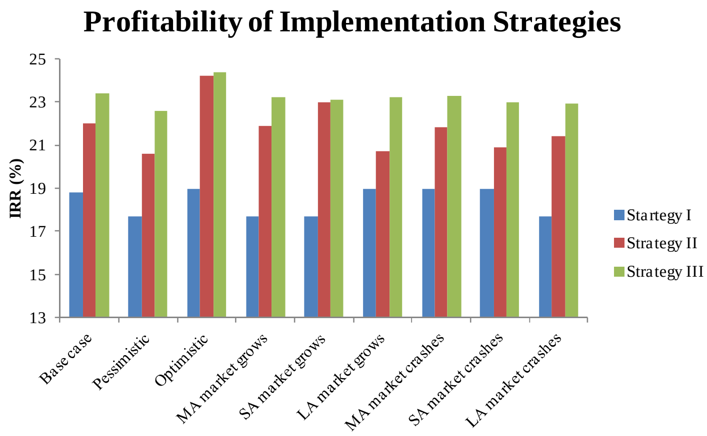

Figure 9. Profitability of Implementation Strategies

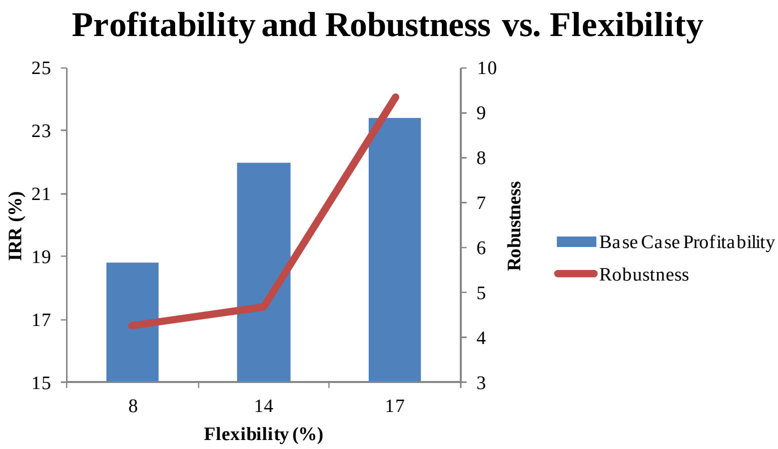

Figure 10. Base-case Profitability and Robustness vs. Flexibility

Figure 11 illustrates the sensitivity of downside IRR on product and fuel price. The difference between strategies in terms of their sensitivity is tremendous. Strategy I can cope with feedstock price increase up to $15/Ton, while this amount for strategy II and strategy III is $30/Ton and $35/Ton, respectively. The same trend can be seen for sensitivity on fuel price. An increase of $150/Ton in fuel price pushes strategy I into the range of low profitability, while $250/Ton and $300/Ton increase in fuel price will have the same effect on strategies II and III, respectively.

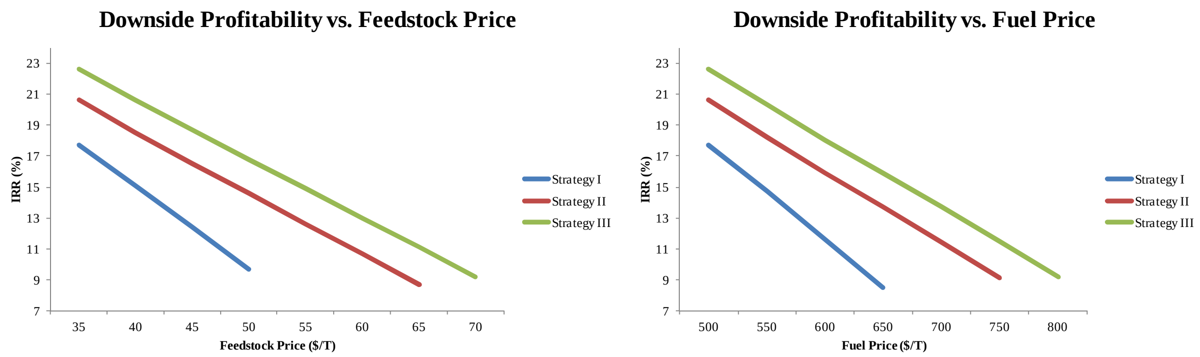

Figure 11. Sensitivity analysis on feedstock and fuel price

A Monte Carlo analysis was done on feedstock price and product prices. The price distributions are presented in Figure 12. The results are shown in Table 6 and Figure 13.

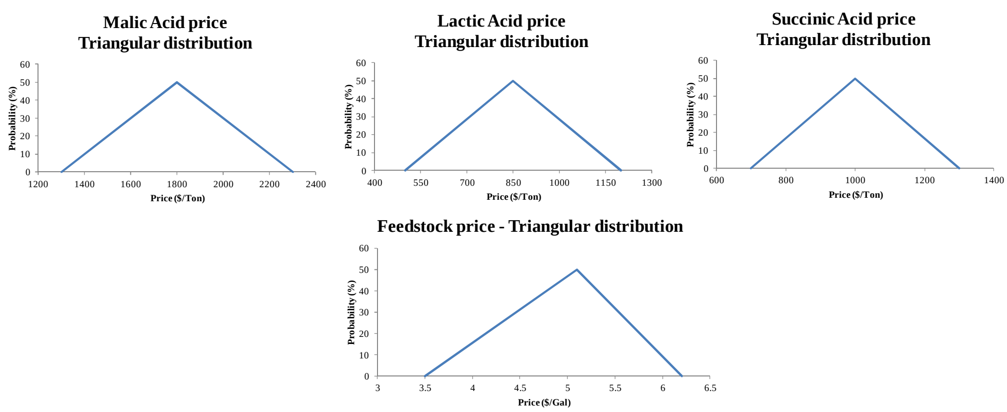

Figure 12. Price probability distributions

Table 6. Result of Monte Carlo simulation

Strategy	IRR (%)	Standard deviation (%)
Strategy I	18.8	13.9
Strategy II	21.9	9.3
Strategy III	23.3	8.9

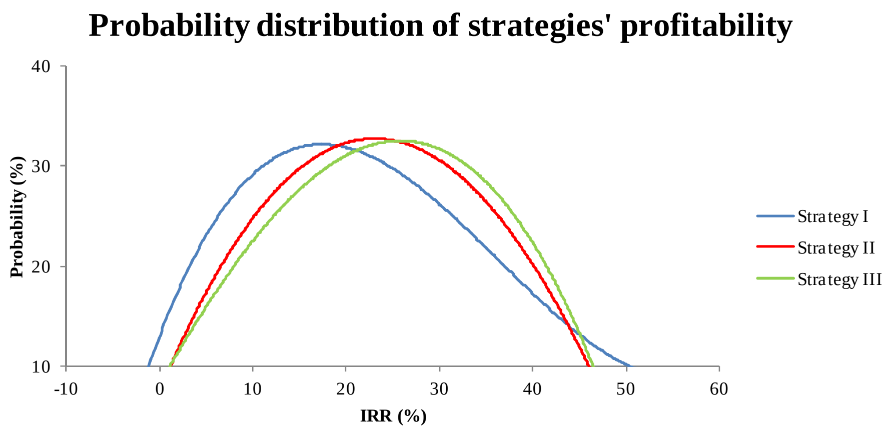

Figure 13. Probability distributions of IRR

The result of Monte Carlo simulation is consistent with the results presented before. The profitability of strategy III is the highest. Moreover, the standard deviation of the calculated IRRs for this strategy has the smallest value, which connotes that strategy III is the most robust strategy among others. This supports the claim that when flexibility increases, the robustness of the system improves.

Lastly, the sensitivity of the system to the aspects related to process integration was studied. Figure 14 demonstrates that IRR is quite sensitive to the percentage of extracted hemicelluloses. The reason is that the extracted percentage is directly related to xylitol production yield. Xylitol is highly value-added and comprises around 25% of net revenue. Figure 15 shows how sensitive the IRR is to percentage of lignin separation. Separated lignin is used as fuel. Thus, decreasing the yield of lignin separation results in increasing the amount of fuel required for energy production.

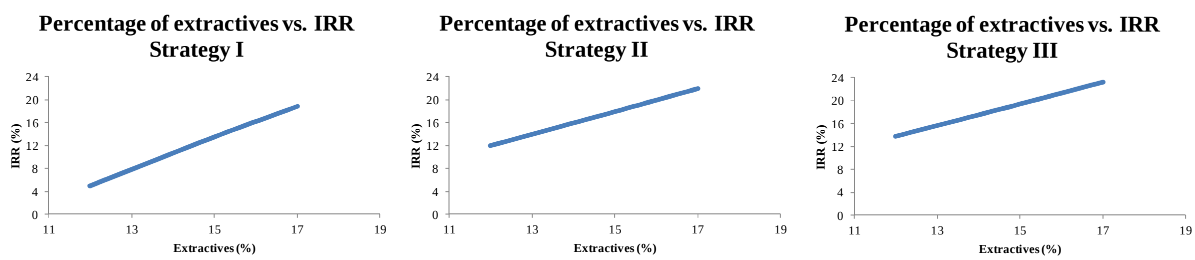

Figure 14. Sensitivity to extractives percentage

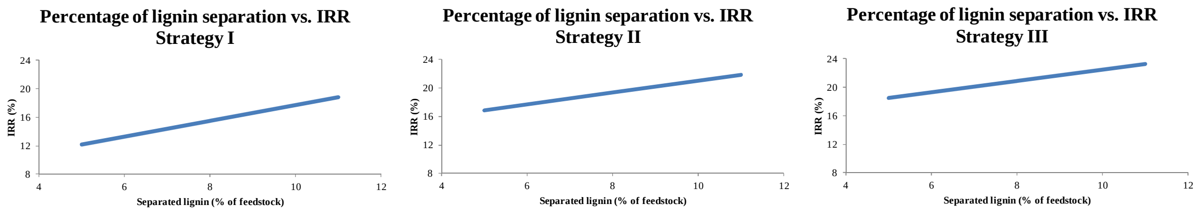

Figure 15. Sensitivity to lignin separation

Conclusion

The result of phased implementation analysis shows that proposed strategies to make the system more flexible over the long term are more profitable than the strategy which implements the least flexible configuration. The effect of flexibility on lowering the sensitivity of the system's profitability on feedstock, energy, and product prices is considerable. The ability of shifting from a less profitable product to a more profitable one enables reducing the sensitivity on product price. Moreover, flexibility increases the cash flow of the company and thus makes it less vulnerable to price changes. Via the phased approach, the capital spending is divided into three phases. 45% of capital spending is done in the first phase, 47% in the second phase and the rest in the third phase. This will help the company in coping with lack of capital.

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APPENDIX F – Conference Paper: Integrating product portfolio design and supply chain design for forest biorefinery

INTEGRATING PRODUCT PORTFOLIO DESIGN AND SUPPLY CHAIN DESIGN FOR THE FOREST BIOREFINERY

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Abstract

Supply chain (SC) design involves making strategic decisions for the long term, e.g. location and capacity of facilities, flow of material between SC nodes, as well as choosing suppliers and markets. The forest biorefinery is emerging as a promising opportunity for improving the business model of forest product companies, however introduces significant challenges in terms of mitigating technology, economic and financial risks – each of which must be systematically addressed, including in SC design. In this regard, product portfolio definition and technology selection are two important decisions that have rarely been considered in a systematic SC evaluation. This paper presents such a methodology, in which product/process portfolio design and SC design are linked in order to build a design decision making framework. According to this methodology, "manufacturing flexibility" links product/process portfolio design to SC design, through a margins-centric SC operating policy. Techno-economic studies and advanced cost modeling along with scenario generation for price changes representing market volatility are employed in the methodology.

Keywords

Forest Biorefinery, Supply Chain Design, Product Design

Introduction

Pulp and Paper (P&P) companies in Canada are facing a stalemate situation (Stuart, 2006). Their business has been endangered by global low-cost competitors; therefore they are encountering declining markets and over capacity. In order to remain low-cost producers, they have cut R&D activities and spent minimum capital to modernize their mills and thus they are dealing with the lack of knowledge of product quality requirement and supply chain (SC) practices. Enterprise Transformation (ET) has been proposed by experts as a solution for rescuing Canadian P&P industry from its current situation (Chambost et al., 2008a). ET implies evolving aggressive corporate-wide initiatives designed to impact the strategies, structures and human system of the corporation – as well as to create more sustainable and profitable organizations. ET must be performed in two broad separate ways referenced as "inside-out" and "outside-in". Inside-out transformation is when the current mission/vision of the company is kept unchanged and the company is made-over in terms of its processes and manufacturing culture. Outside-in transformation involves changes in current mission/vision and the core business of the company

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by producing new products and providing new services. What helps P&P companies to transform their enterprise and to rescue their industry is the Forest Biorefinery (FBR). P&P companies have some competitive advantages, e.g. access to biomass and engineering know-how, established infrastructure close to forest biomass and established SC for wood, pulp and paper. Hence, taking advantage of these privileges, P&P companies can transform their enterprise by implementing the FBR, because, in order to implement the FBR, companies must produce bioproducts besides pulp and paper, which implies outside-in transformation. On the other hand, FBR implementation will change company's core business; therefore they need new management practices and manufacturing culture, which address inside-out transformation.

FBR implementation can be performed based on a phased approach which can be considered by P&P companies, Figure 1(Chambost et al., 2008 a).

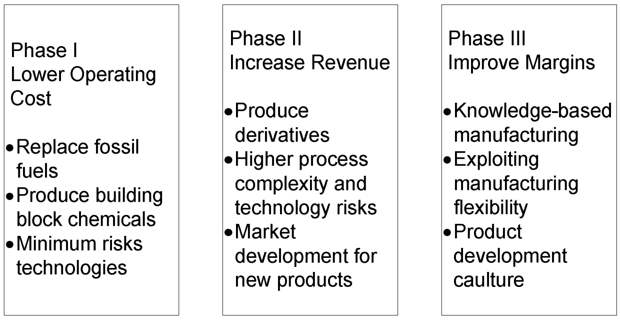

Figure 1. Strategic implementation of the biorefinery by a P&P company

In phase I, companies must lower their operating costs by producing substitute fuel products for fossil fuels such as bunker C or natural gas, or by employing new technologies with minimum risks. Such projects must compete internally for capital due to lack of capital spending budget in P&P companies. In phase II companies must increase their revenue by producing added value products. This phase includes change in the core business, which in turn implies outside-in transformation. Considering that phase II requires capital, new technology and new product delivery requirements, partnership is of crucial importance in this step. Therefore the main challenge at this phase is to select the most sustainable product/process portfolio and partner(s). In phase III companies must focus on improving margins by exploiting manufacturing flexibility through "knowledge-based manufacturing". This latter term implies advanced SC optimization techniques which identify the trade-offs between supply, demand and manufacturing capability via advanced cost accounting techniques and improve the company's margin by SC optimization given the manufacturing capability of the mills. As these activities seek improved bottom-line results via transforming the enterprise in terms of work and process steps, phase III implies an inside-out transformation (Chambost et al., 2008 a).

Producing several products implies the opportunity of taking advantage of manufacturing flexibility via the identification of product portfolios at a given mill, i.e. integration of biorefinery product families based on key building blocks and their related derivatives with existing P&P production (Chambost et al., 2008 a). Thus according to the feedstock and product price as well as supply and demand constraints the manufacturing flexibility can be exploited to produce different products with different rates in order to optimize the company's margin. Hence, the challenge in phase III is to design the SC network and to manage it given the manufacturing flexibility needed for improving the margins. The SC should be uniquely designed in order to provide a competitive advantage over the long term while supporting value chain creation and/or maximization. In this regard, developing a SC-based analysis, which can explore the manufacturing flexibility, is of crucial importance. Laflamme-mayer et al. showed how such an analysis contributes to margin improvement for a P&P mill. Their proposed SC-based analysis first identifies the cost structure of the mill by means of a cost model and then analyzes the results by a multi-scale SC optimization framework. The proposed analysis enables reflecting the manufacturing capability of the mill at the SC-level decision making (Laflamme-Mayer et al., 2008). Same approach can be employed for analyzing the manufacturing flexibility capability of the FBR in the SC-level decision making.

Given the phased approach presented above, there are two critical aspects for the FBR implementation, i.e. product/process portfolio definition related to phase II and SC network design related to phase III. What links these two aspects is "manufacturing flexibility". Manufacturing flexibility is the capability of producing different products with different rates based on the product price with the goal of mitigating risks associated with market volatility and stabilizing the margins. This type of flexibility is inherent in the process design, because the process must be designed in such a way that enables exploiting the flexibility. Therefore, product/process portfolios are defined for flexibility to stabilize the margins and to secure the return on investment. Afterwards, the range of manufacturing flexibility is established as a design target and then this established target is designed. Finally the SC network is designed so that the market requirements can be met through the designed SC network and within the designed range of manufacturing flexibility. The goal of this paper is to propose a hierarchical methodology for SC-based analysis which can integrate these three aspects, i.e. product/process portfolio design, design of manufacturing flexibility, and SC network design. The proposed methodology will be able to evaluate product/process portfolio options and the required manufacturing flexibility, and to reflect them in the SC network design.

Integration of product, process and SC design has not gained attention in the chemical engineering context. The majority of articles in the body of literature relate to assembly process environments, e.g. car manufacturers and electronics manufacturers. Huang et al. (2005) addressed the challenge of designing effective supply chain systems that integrate platform product decisions, manufacturing process decisions, and supply sourcing decisions for a product family of notebooks. Blackhurst et al. (2005) proposed a methodology, called Product Chain Decision Model (PCDM), whose objective is to model complex and dynamic systems, such as supply chains, and the decision-making processes inherent in the operation of the supply chain, product and process design decisions. An aviation electronics provider was studied as the industrial case. Fixson (2005) introduced product architecture as a tool to link product, process and SC design decisions for assembly processes. Lamothe et al. (2006) developed an optimization model for selecting a product family and designing its SC for car manufacturers.

In the context of biorefinery, Sammons et al. (2008) proposed a general systematic framework for optimizing product portfolio and process configuration in integrated biorefineries. The framework first determines the variable costs as well as fixed costs using data in terms of yield, conversion and energy usage for each process model. Then, if a given process model needs the use of solvent, molecular design techniques are used to identify alternative solvents that minimize environmental and safety concerns. Next, process integration tools, e.g. pinch analysis, are employed to optimize the models. Lastly, the optimized model will generate data for economic and environmental performance metrics. An optimization formulation enables the framework to decide whether a certain product should be sold or processed further, or which processing route to pursue if multiple production pathways exist for a special product.

The hierarchical methodology presented in this article can be differentiated from the framework proposed by Sammons et al. in the following ways: (i) It seems that their methodology does not involve market investigations before selecting the products. (ii) Also no SC metric exist in the framework. (iii) The definition of flexibility in the methodology presented in this work is different, i.e. manufacturing flexibility, which is inherent in the design and enables to produce different products with different rates, versus flexibility in choosing products and process.

Methodology

The hierarchical methodology proposed in this paper comprises three major steps each of which points out one of the three key aspects mentioned above, i.e. product/process portfolio design, design of manufacturing flexibility, and SC network design. The first step deals with product/process portfolio design through product portfolio definition and Large Block Analysis (LBA). The second step implies establishing the design target of the manufacturing flexibility and then designing the established target. The third step addresses the SC network design which involves redesigning the SC network configuration.

First Step: Product/Process Portfolio Design

At this step, the challenge is to identify the most promising product/process combination from a large range of product/process opportunities (Werpy & Peterson, 2004). Therefore this step can be divided into two consecutive parts; (1) product portfolio definition, (2) LBA for the defined product portfolios in order to generate product/process portfolios.

The selection of the most promising product portfolio includes two major concepts:

(i) First, the product identification is based on a market-driven analysis reflecting the commercial product opportunities. In this regard, products could be classified into three groups; (a) Replacement products which are identical in chemical composition to the existing products in the market, but made out of renewable feedstock, e.g. biopolyethylene. (b) Substitution products which have different chemical composition, but the same functionality, e.g. polylactic acid (PLA) instead of polyethylene terephtalate (PET). (c) Novel products like biomaterials, nanocomposites which have new functionalities and therefore no existing markets (Chambost et al., 2008 a).

(ii) The product portfolio of a mill should be the expression of value creation via the determination of key building block offering high potential for added-value products and the integration of the new identified products with traditional P&P products (Chambost et al., 2008b). Important elements should be considered while considering the definition of portfolios such as follows; (a) Manufacturing flexibility is an important criterion for product portfolio definition. It must be investigated that which set of products introduces a better potential for flexibility. (b) The defined product portfolio must be able to stabilize the margins and to secure the return on investment (ROI), thus market volatility, legislation changes and other factors must be taken into consideration. (c) The definition of product portfolio should take into account the identification of sustainable partnership models, i.e. partnering with technology providers and/or chemical companies, in order to secure the SC and lower the risks of entering an existing/new value chain.

Product Portfolio Definition

A three-stage methodology has been developed for the definition of product portfolio, Figure 2 (Chambost et al., 2008 a). In the first stage sets of possible products must be identified. For this purpose, overall product opportunities are investigated based on market, economic and product specific information such as product functionalities, volume, market size and growth, market saturation and basic margins. The goal of this stage is to identify a list of promising bioproducts. In the second stage, based on market and competitiveness criteria and a preliminary techno-economic study, possible sets of product families can be identified. Product families comprise bioproducts that link to each other via common processing steps. For instance, ethanol, ethylene and polyethylene could form a biorefinery product family, since ethanol can be converted into ethylene and further into polyethylene. At the last stage, according to a mill or company-based analysis, product portfolios will be generated. Product portfolios are the combination of existing P&P products and new biorefinery products. At this stage, mill’s specifications must be taken into consideration in order to identify the opportunities for integration between P&P processes and bioprocesses in terms of feedstock, chemicals and energy. Finally a critical risks assessment is conducted for each product portfolio.

Large Block Analysis (LBA)

The objective of LBA is to provide comparable techno-economic data such as operating cost, capital investment cost and profitability, of different product/process portfolios and then to screen out non-profitable portfolios.

LBA has seven major stages which are shown schematically in Figure 2.

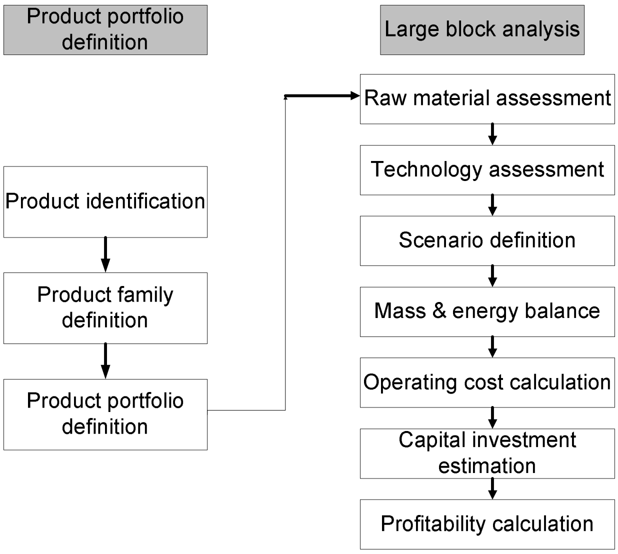

Figure 2. Product/Process portfolio definition

At the first stage, which is "raw material assessment", given the defined product portfolios, list of raw materials must be identified based on their accessibility to the mills and the maximum available volume according to their cost. The second stage is "technology assessment" in which emerging technologies for producing each product must be surveyed, taking into account the mass and energy balance, type of feedstock and technological risks of each technology. At the third stage, called "scenario definition", the combinations of raw material/process/product are generated as scenarios. From raw material to product, there are different pathways and several processing routes. For example, as shown in Figure 3, for producing bioethanol from biomass, there are two pathways, i.e. biochemical and thermochemical. For each of these pathways, different types of process can be used, such as gasification for thermochemical pathway, and enzymatic or acidic hydrolysis for biochemical pathway. Finally there are many technology providers for each process. Therefore each scenario includes one type of feedstock, a specific pathway, processing route and a technology provider related to the processing route, and finally a product. Thus, to define scenarios, given the outcome of the last two stages, i.e. raw material and technology assessment, the specific technology provider, and hence its corresponding process type and pathway, and the required raw material for producing each product must be identified. At this stage, the potentials of integration of selected portfolios with the existing mill must be taken into account in terms of technological fit, integration factors and risks.

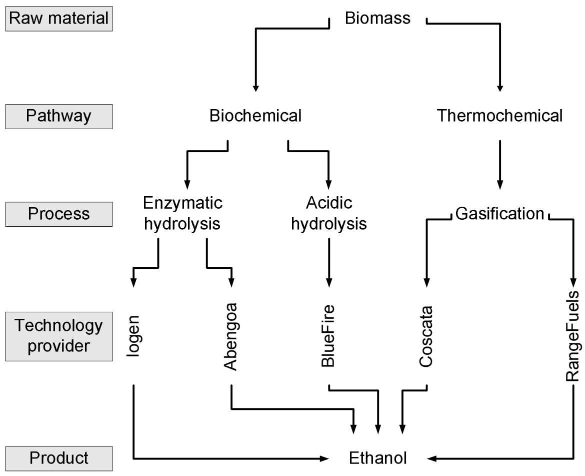

Figure 3. Chemical pathways from raw material to ethanol

At the fourth stage, "mass and energy balance" is done for each scenario based on technology provider's and raw material specific information. The fifth stage deals with "operating cost calculation". There are two types of operating costs: variable and fixed cost. Variable costs such as costs of chemicals, fuels, etc. are calculated based on the balance sheets of the processes and price information. Fixed costs involve labor cost, maintenance, insurance and taxes, and general overhead. The sixth stage is "capital investment estimation", in which capital investment is estimated for each scenario based on published information for stand-alone bioprocesses. Then the mill's impact will be investigated in order to identify the potentials for integration with P&P processes in terms of chemicals or energy. In this regard, the existing mill system that can be used for the bioprocesses must be defined and afterwards, based on the demand of the bioprocesses and the current mill specifications, the cost of modification needs of the mill system can be estimated. In the last stage, which is "profitability calculation", the profitability of each scenario according to the revenue from end products and by-products will be estimated by means of profitability measures such as NPV, IRR or ROI. After these stages, the non-profitable scenarios will be screened out and a finite number of scenarios will be selected as product/process portfolios. These portfolios will be analyzed further so that the best portfolio can be identified.

Second Step: Designing the Manufacturing Flexibility

This part of the methodology contains two steps which must be implemented for the remaining product/process portfolios; in the first step the range of flexibility is established as a design target for each process and in the second step the established target of each process is designed. In order to perform this part of the methodology, two tools are needed; (1) a SC model, (2) an operations-driven cost model. SC model aims to maximize the profitability across the entire SC by first identifying the trade-offs between the demand and production activities and then by finding the optimal alignment of manufacturing capacity and market demand. On the other hand, the operations-driven cost model is based on “operations-driven” thinking, which implies using lower-level process data and detailed process analysis in order to better reflect manufacturing capability for higher-level decision-making. Hence, the overall objective in operations-driven thinking is first to characterize the manufacturing operations (descriptive) by identifying the cost drivers and second, to provide advanced decision support (prescriptive) (Janssen et al., 2006).

SC Model

The SC model aims to calculate the optimum profitability of the whole SC. It is formulated into an optimization problem whose objective function is the sum of revenues from different main products and by-products subtracted by SC costs including feedstock cost, inventory cost, production cost, transitions and shutdowns cost. There are two types of decision variables in the mathematical formulation of the SC model. The first type is continuous variables which comprise flow of material between SC nodes, e.g. flow of feedstock from suppliers to the mill, amount of each product that must be produced, and the inventory levels for each type of feedstock and product. The second type is binary variables which imply “yes/no” type of decisions, e.g. which product must be produced or which production line must operate. Each node of the SC, i.e. suppliers, inventories, manufacturing centers, has its own constraints which must be formulated mathematically.

Operations-Driven Cost Model

The operations-driven cost model is where cost and process information are captured and systematically integrated to characterize the processes (Janssen, et al., 2006). Cost model must be made up for all remaining product/process portfolios from previous step of the methodology. The outcome of the cost model are manufacturing costs for each design alternative (see *Designing the Established Target*), as well as profitability measures based on capital and manufacturing costs, which in this methodology will be ROI. The cost model is fed, from one side, by process information which represents the resource consumption, and on the other side, by cost information which shows the cost of each resource. Each mill is represented by a number of Process Work Centers (PWC) in which some processes are performed. The cost incurred by the processes in each PWC is calculated. Also there is an Overhead Work Center (OWC) which introduces the manufacturing overheads and non-manufacturing costs. These costs are used to calculate the final cost object, which can be the product cost for each design alternative.

Establishing the Range of Manufacturing Flexibility

For each process in each portfolio, there is a nominal production rate based on the result of “technology assessment” step of LBA. At this stage, the range of flexibility within which the manufacturing processes must operate is determined. In other words, it must be determined that, given the price volatility in the market and with the aim to maximize the profitability, to what extent each production rate must be able to vary. For this purpose, a finite number of price scenarios, representing the price volatility, are generated. It is worth mentioning that price volatility, which implies the future market situation, is modeled through aforementioned scenario generation with the aim of long-term strategic decision making. Thus product prices won't be taken in real time. Real-time analysis will be performed at tactical and operational levels which deal with the dynamic aspect of the SC. After generating price scenarios, the SC model is run for each scenario with no constraint on the rate of manufacturing processes, so that the SC model can find the optimum production rate for each process based on the product price. Figure 4 shows an example.

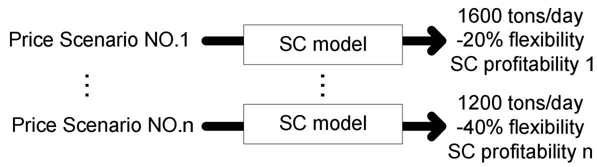

Figure 4. SC model input and output

Considering that the nominal production rate is 2000 tons/day, given a decrease in product price scenario NO.1, the optimum production rate obtained by the SC model is 1600 tons/day, which represents -20% of flexibility based on the nominal rate (2000 tons/day), while the obtained result from SC model for the product price NO.n, representing a stronger decrease in price, is 1200 tons/day, which represents -40% of flexibility. This calculation must be done for each scenario, so that it is determined that to what extent each process needs to be flexible for a given price volatility. Also the SC profitability for each price scenario will be estimated and finally based on the range of flexibility and SC profitability the range of flexibility as a design target will be determined.

Designing the Established Target

At this stage, the range of flexibility will be constrained by limiting the production rates based on the result of the previous stage. For instance, given that -40% was the maximum flexibility obtained from the last stage, this percentage will be the flexibility constraint which cannot be exceeded. In other words, the SC model won't be able to go beyond this range. For this stage, a limited number of design alternatives will be generated to represent the flexibility. As it is impossible to have -40% of flexibility on a continuous process, therefore in order to have this percentage of flexibility, the production line must be divided into 2, 3 or 4 lines whose sum of production rates is equal to the nominal rate (2000 tons/day). Figure 5 shows an example.

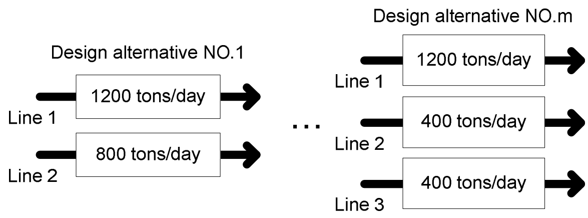

Figure 5. Design alternatives

As shown in Figure 5, the nominal rate (2000 tons/day) can be represented in terms of two parallel lines (1200 tons/day and 800 tons/day, or 1400 tons/day and 600 tons/day) or three parallel lines (one line for 1200 tons/day and two lines for 400 tons/day). Then, for each price scenario, the SC model will be run and the SC profitability as well as ROI will be calculated for each design alternative. Therefore, for each design alternative, a set of SC profitability and ROI will be calculated for a set of price scenarios. Based on these results, the most profitable design alternative will be identified. It must be mentioned that these steps must be performed for all remaining portfolios, so that the best design alternative for each portfolio can be delineated. Figure 6 shows this stage graphically.

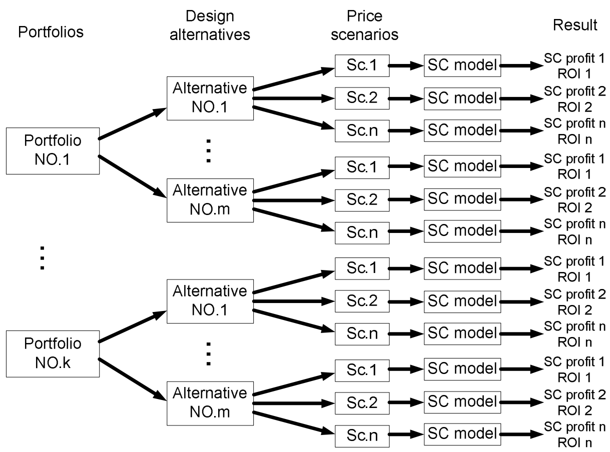

Figure 6. Identifying the most profitable design alternative

Third Step: SC Network Design

The goal of this step is to design the SC network for each portfolio. For this purpose, a finite number of SC network alternatives will be generated for each portfolio. Figure 7 shows this step graphically. SC network alternatives can be defined in terms of expansion of existing facilities or buying new facilities in different areas. Then, given the same price scenarios, SC model will be run for each SC network alternative and the SC profitability will be calculated for each of them. Based on the results, the best SC network alternative can be determined for each portfolio.

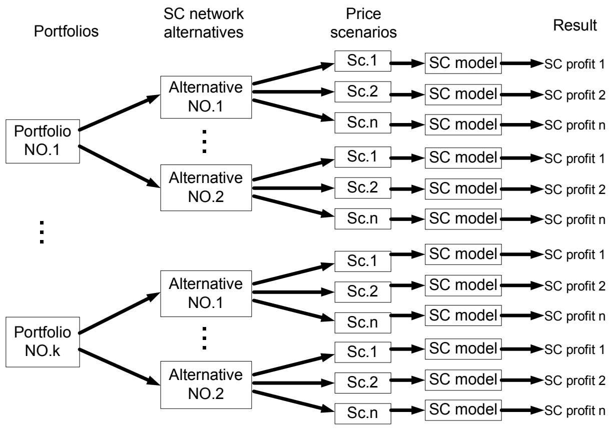

Figure 7. SC network design alternatives

Decision making framework

As it was mentioned previously, the proposed methodology must be performed for all portfolios. After implementing this methodology, each portfolio can be characterized by means of several aspects, i.e. manufacturing flexibility, SC profitability and ROI. These aspects can be used as different metrics in a multi-criteria decision making framework. It is worth mentioning that all of these metrics would be SC metrics. Another type of metrics can be provided by Life Cycle Analysis (LCA) and added to the framework. Based on the result obtained by the multi-criteria decision making framework the best product/process portfolio can be determined.

Illustrative example

This methodology will be applied in a case study at a P&P mill. This P&P mill, which produces one grade of pulp and one grade of paper, aims to implement the FBR by producing bioproducts. After product market analysis, two product portfolios are considered; the first portfolio includes the two grades of pulp and paper plus ethanol and ethylene, while the second portfolio contains the same pulp and paper grades plus lactic acid (LA) and poly lactic acid (PLA). Different companies provide the technology for production of such products. If, based on the characteristics of the existing P&P mill, two scenarios for each product portfolio can be considered, four product/process portfolios can be defined. After carrying out mass and energy balances for each scenario, the profitability of each scenario is obtained by calculating the operating and investment costs. The two most profitable portfolios are retained for the next step. Assuming that one portfolio involving ethanol/ethylene and one including LA/PLA are selected, in the next step the range of required flexibility must be determined and six price scenarios are generated for each portfolio, as shown in Table 1.

Table 1. Price change scenarios

		1	2	3	4	5	6
Portfolio 1	Ethanol	-	↓	↓	-	↓↓	↓↓
	Ethylene	↓	-	↓	↓↓	-	↓↓
Portfolio 2	LA	-	↓	↓	-	↓↓	↓↓
	PLA	↓	-	↓	↓↓	-	↓↓

The first two scenarios consider a price decrease for only one of the products, while third scenario represents price decrease for both products, e.g. ethanol and ethylene. The next three scenarios follow the same rule, but consider a stronger decrease in product prices. All scenarios are defined using price decreases in order to address the worst case. For each of these scenarios, the developed SC model is run without constraint on production capacity in order to obtain the optimal production rate of each process for each scenario, and to determine the flexibility range. Given the number of retained product/process portfolios and price scenarios, i.e. two and six respectively, the SC model must be run twelve times. Table 2 shows the range of flexibility needed for each process in the case of each scenario realization.

Table 2. Range of flexibility for each process

	1	2	3	4	5	6
Ethanol	0	-15	-20	0	-23	-30
Ethylene	-10	0	-5	-20	0	-14
LA	0	-10	-14	0	-13	-20
PLA	-8	0	-3	-10	0	-7

Therefore, -30%, -20%, -20% and -10% of flexibility are the maximum flexibility needed for ethanol, ethylene, LA and PLA production processes, respectively. In the next step design alternatives are defined based on calculated ranges of flexibility. For each process, two alternatives have been considered. Given that the nominal production rate for ethanol/LA and ethylene/PLA is 2000 tons/day and 1000 tons/day, respectively, the design alternatives are defined as presented in Table 3.

Table 3. Design alternatives for each portfolio

		Design 1	Design 2
Portfolio1	Ethanol	2 lines: 600 tons /day 1400 tons/day	3 lines: 300 tons/day 300 tons/day 1400 tons/day
	Ethylene	2 lines: 200 tons/day 800 tons/day	2 lines: 200 tons/day 800 tons/day
Portfolio2	LA	2 lines: 400 tons /day 1600 tons/day	3 lines: 200 tons/day 200 tons/day 1600 tons/day
	PLA	2 lines: 100 tons/day 900 tons/day	2 lines: 100 tons/day 900 tons/day

Figure 8 illustrates the ROI of each design alternative for each price scenario.

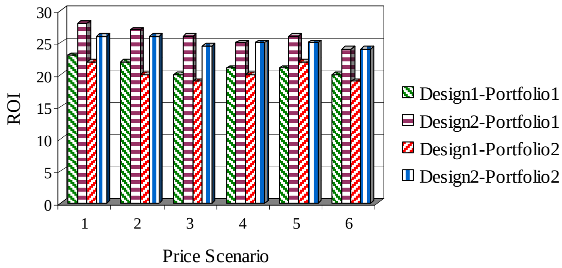

Figure 8. ROI of design alternatives for each price scenario

According to the resulting ROIs, design 2 for both portfolios is a better choice. Therefore, for the next step, which deals with SC network design, two SC network alternatives are defined for each of these design alternatives. These network alternatives are presented in Table 4.

Table 4. SC network alternatives

Alternative 1	Alternative 2
Expanding the existing warehouse	Buying a new warehouse

Again the SC model is employed to calculate the profitability of these SC network alternatives for each portfolio. Eventually, the final result, SC profitability, range of flexibility and ROI, will be used as SC metrics, along with LCA metrics, in a multi-criteria decision making framework. The final result of this framework will determine the best product/process portfolio.

Conclusions

A hierarchical methodology is proposed to integrate product/process portfolio design, design of manufacturing flexibility, and SC network design. SC optimization, techno-economic study and operations-driven cost modeling are employed as tools. Scenario generation is used to address the product price volatility. Inspired by work done previously in Environmental Design Engineering Chair at Ecole Polytechnique in Montréal regarding SC-based analysis in the context of P&P industry, this methodology shows how the FBR can be implemented strategically via a step-wise approach. Through this step-wise approach, different options in terms of product/process portfolio can be studied and their potential for flexibility can be investigated. Also, the best SC network for these options can be identified. Therefore product portfolio design and process design can be reflected in the SC strategic design via this SC-based analysis.

Acknowledgments

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APPENDIX G – Conference Paper: Scenario-based strategic supply chain design and analysis for the forest biorefinery

Scenario-Based Strategic Supply Chain Design and Analysis for the Forest Biorefinery

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Abstract

Supply chain (SC) design involves decisions for the long term, e.g. number, location and capacity of different SC nodes, production rates, flow of material between SC nodes, as well as determining suppliers, markets and partners. The forest biorefinery (FBR) is emerging as a new possibility for improving forestry company business models, however introduces significant technological, economic and financial challenges - which can be systematically addressed in strategic SC design. This paper presents a scenario-based approach to strategic SC design for the FBR, designing the SC based on the impacts of the design on tactical-operational SC activities. Two kinds of scenarios are used; market scenarios representing market volatility and SC network scenarios (alternatives) representing different biorefinery options/strategies. The SC analysis evaluates SC alternatives for the case of different market scenario.

Keywords: Forest Biorefinery, Supply Chain, Partnership, Scenario-Based Approach

8. Introduction

In the design of a SC, long-term decisions should be made, i.e. products, technologies, number, location and capacity of each facility, e.g. plants, warehouses and distribution centers, and the target markets [1]. In a practical problem, it is difficult to address such decisions in an optimization problem, because they are linked to aspects that cannot be modelled, e.g. understanding the market and market strategies, emerging products and processes, the capabilities of the existing assets of the SC, and the potential partners. It is thus preferable to pursue a systematic methodology that addresses these factors in a step-wise manner. The

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methodology which is presented in this paper, seeks a set of feasible biorefinery options, not the best one, which a company can strategically pursue considering practical aspects. Many of these aspects can be addressed in different scenarios instead of being modelled into an optimization formulation. This scenario-based methodology results in a set of solutions. A multi-criteria decision making (MCDM) framework can subsequently be used to find the best option from the company point of view. In order to execute this step-wise methodology, certain decisions must be made via integration with other methodologies, i.e. product portfolio definition to determine the set of products, techno-economic study to choose technologies to produce the targeted products. What will be determined by the scenario-based approach is the SC network design including the number, location and capacity of warehouses and distribution centres as well as partners to collaborate with.

8.1. *Problem definition*

A forestry company wants to implement the biorefinery by examining the portfolio of products which secure profit, using processes which enable better response to volatile market conditions, and companies with which a partnership can be made. On one hand, market conditions must be taken into consideration, and on the other hand, possible process/SC options to be implemented must be identified. Scenario generation is used to address both aspects. Market conditions are reflected into the problem via market scenarios. Also, possible biorefinery options, each implying specific implementation strategies, are made in terms of alternatives, each of which includes a product portfolio, a technology for the production of each product, and a SC network for each portfolio. In this paper, SC network alternatives are defined and combined with product/process portfolios. A margins-based SC optimization model calculates the profitability of each combined alternative, i.e. a biorefinery option, in case of market scenario realizations.

The SC network must be designed in way such that, by optimizing the tactical-operational SC activities, SC profit is maximized. As a result, this approach evaluates the SC network based on the impacts of the design on tactical-operational activities. The margins-based optimization model takes advantage of the flexibility of processes, and chooses orders and schedules production so that profit is maximized.

8.2. *Margins-based optimization*

The operating policy in the pulp and paper (P&P) industry is said to be “manufacturing-centric”, i.e. the management focus is on capacity planning [2] assuming that minimizing production costs will result in the highest profitability [3]. Also, production planning assumes known orders and a fixed sequence of grades, no matter what the price and demand are. For the FBR, the operating policy would ideally shift to a margins-based approach, which maximizes profit over the entire SC [3]. In this approach, long-term contracts and short-term order selection are made with respect to not only process/production constraints, but also inventory and transportation constraints. Given the number and length of time intervals, price and demand data, capacity data, and direct cost parameters, the main decision variables to be determined for each time interval include; contracts to make, orders to fulfil, amount of feedstock, amount of products to be produced, flows of material between SC nodes. The objective function is the SC profit, involving revenue as well as production, inventory, transportation and changeover costs.

8.3. *Manufacturing flexibility*

Today’s market is subject to significant volatilities in terms of price and demand. To mitigate risks against such uncertainties, it is of crucial importance to enhance the reactivity and proactivity [4] implying flexibility. In the chemical engineering context, four flexibility types have been studied widely; recipe flexibility, process flexibility, product flexibility, and volume flexibility [5]. An FBR is able to produce several products, i.e. P&P products, bio-products and energy. Given feedstock and product price, supply and demand, product/volume flexibility can be exploited to maximize profit. The company should analyze its access to feedstock, product price, as well as orders/demands and find the alignment between demands and its capacity [5].

9. Scenario-based approach for the strategic design of the SC network

The methodology proposed for scenario-based SC network design is shown in Figure 1.

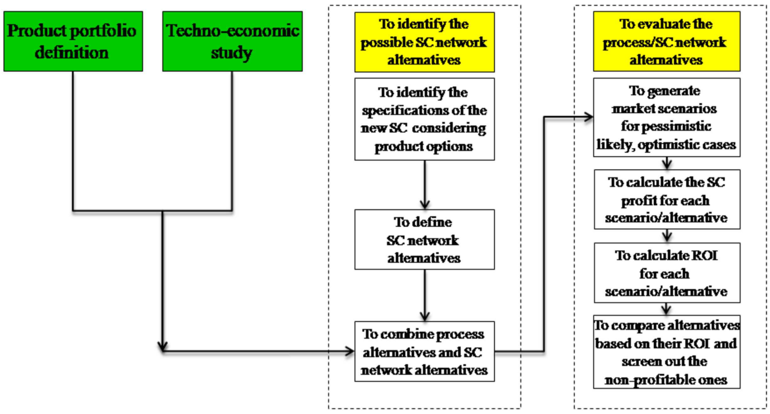

Figure 1. Scenario-based methodology for the SC network design

Product/Process portfolios are inputs. The methodology includes two parts; first possible SC network alternatives are identified and after being combined with product/process portfolios, product/process/SC network alternatives are evaluated based on their performance at the operational level. An illustrative example is presented to concretize the methodology. Two portfolios, A & B, are defined [6]. In A, Fischer-Tropsch liquids (FTL) are produced and separated into waxes and diesel. Then diesel is converted to jet fuel (JF). In B, butanol, succinic acid (SA) and lactic acid (LA) are produced. Process alternatives for each portfolio are shown in Figure 2. Each alternative represents a specific level of flexibility in terms of product and throughput. In A1and A2, diesel is converted to JF completely and by half, respectively. A3 can be used in both ways. In B1, SA and LA are produced in fixed volumes, while in B2, an extra recovery system for SA and LA enable doubling the production of one at a time.

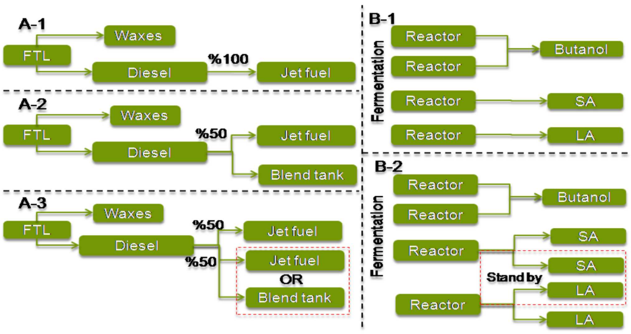

Figure 2. Process alternatives for each portfolio

9.1. *Identifying possible SC network alternatives*

9.1.1. *Identifying the specifications of the new SC considering product options*

Forestry company SC networks are in place with their existing assets. Some processing steps/facilities are common among processes in the mill and thus similar facilities and assets can be employed or redesigned when implementing the biorefinery. It should be investigated how facilities should be modified or added to enable the mill to process more biomass. Also, each product has specific properties which have related facilities for transportation and storage.

9.1.2. *Defining SC network alternatives*

Based on the Problem specifications, several SC network alternatives can bedefined which reflect the requirements of the new SC network. The issues to be addressed are;

- Partnership: Partners can cooperate in providing technology, delivering the product, buying and/or selling the product. In this way, some or all of the partner's SC assets are utilized and less capital is needed for the combined SC network.
- Location and capacity of distribution centers: based on the location of the plant, several target markets might be around the plant. Thus, different distribution centers with different capacities can be assigned to target markets.
- Transportation network: Based on the characteristics of the products, different ways of transportation, either by the company or via contract with other companies, can be utilized for product delivery. Examples of alternatives for case study portfolios are shown in Table 1.

Table 1. SC network alternatives defined for each portfolio

Alternative A-1	Alternative A-2 A-3	Alternative B-1	Alternative B-2
Waxes: Partnership JF: on spot	Waxes:Partnership JF & diesel: on spot	BuOH, SA, LA: Partnership	BuOH: Partnership SA & LA: on spot
Buy trucks	Contract for transportation	Buy trucks	Contract for transportation

9.1.3. *Combining process alternatives and SC network alternatives*

After defining the SC network alternatives, the capital investment required to redesign the SC network is calculated for each alternative and is added to the capital investment needed for the process technologies. Each combined alternative involves a process configuration with a targeted flexibility level and a SC network related to the products.

9.2. *Evaluating the process design/SC network alternatives*

9.2.1. *Generating price/supply/demand scenarios*

In order to address market uncertainty, market scenarios representing a specific condition in the market with respect to feedstock availability, product demand, and feedstock and product price are generated for pessimistic, likely and optimistic market price cases. For strategic decisions, scenarios are generated for a period of one year.

9.2.2. *Calculating the SC profit for each scenario/alternative*

In this step the SC profit for each alternative is calculated for the case of every scenario. To calculate the SC profit, a SC optimization model is used. The model optimizes the SC profit by determining the orders to fulfil and calculating the optimum value of production rate related to each product and flow of material between SC nodes.

9.2.3. *Calculating the profitability of each scenario/alternative*

In order to evaluate each alternative, the profitability of each alternative should be estimated. In this methodology, return on investment (ROI) is used as the measure of profitability. An example of the final result can be observed in figure 3.

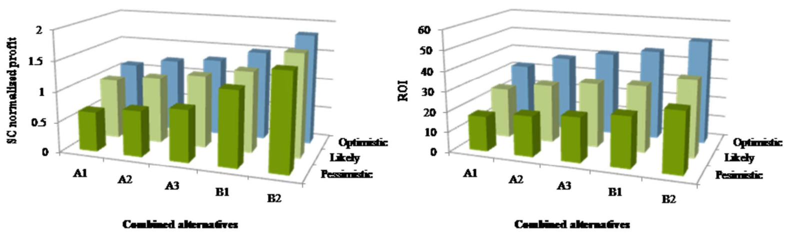

Figure 3. Normalized SC profit and ROI for each combined alternative

10. Conclusions

Biorefinery options involving product portfolio, process configuration and SC network, which can be considered by a company willing to implement the biorefinery can be evaluated using the scenario-based methodology proposed in this paper. By comparing the profitability of alternatives and screening out the non-profitable ones, a set of biorefinery options to be considered can be identified. Our current research focuses on designing and targeting SC flexibility, i.e. designing product/volume flexibility, to make FBR more efficient. In future works, SC robustness will be studied as a key metric for ensuring expected SC profitability in the presence of market uncertainty.

Acknowledgements

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APPENDIX H – Conference Paper: The role of supply chain analysis in market-driven product portfolio selection for the forest biorefinery

21st European Symposium on Computer Aided Process Engineering – ESCAPE 21
E.N. Pistikopoulos, M.C. Georgiadis and A.C. Kokossis (Editors)

The Role of Supply Chain Analysis in Market-Driven Product Portfolio Selection for the Forest Biorefinery

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Abstract

The implementation of the forest biorefinery in retrofit to an existing forestry company requires a strategic shift in the core business from a commodity-driven manufacturing-centric culture, to a margins-driven supply chain culture. In order to diversify the set of traditional forest products to include biorefinery products it is critical to define the associated market and competitive strategies as well as new business models. The penetration of existing mature value chains by replacement and/or substitution biorefinery products requires that supply chain strategies be implemented that create and retain value over the longer term, and secure a unique competitive position. As part of the new product portfolio definition, key supply chain criteria must be identified and considered in the value chain assessment. The role of the supply chain in defining the product portfolio definition and in mitigating risks against price volatility is examined in this paper.

Keywords: Forest biorefinery, product portfolio, value chain, competitive assessment, supply chain

1. Introduction

The forest biorefinery (FBR) is increasingly being considered by forestry companies as a viable business option for diversifying and growing revenues. However designing the biorefinery that serves a promising business model is not obvious. Many possible biorefinery routes can be targeted but only certain of these will bring sustainable competitive advantages and substantial financial reward. The company's biorefinery product portfolio must be systematically identified and the associated technical, techno-economic and commercial risks associated with different options should be determined. For many companies, process design drives the development of the biorefinery, and the question of new product integration into an existing product portfolio is considered through the technology strategy. However for better ensuring the successful implementation of the biorefinery and attracting the interest of strategic investors, a

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robust business model accompanied by a technology strategy that mitigates technical risks is critical. Leading market analyst Roberts [1] identifies four strategic business model elements for attracting strategic investors, being (1) minimal to no technology risks, (2) security and long-term plan for fibre through off-take agreements based on volume and price, (3) a credible business case with specific market strategies, (4) credible financial metrics. The forestry industry, vested in a commodity and manufacturing-centric culture, must be prepared to transform in order to retain value and create margins over the longer term. The unique set of competitive advantages a company may create and maximize through market strategies, including optimization of existing delivery systems and identification of strategic partnerships [2], will be the cornerstone for successful biorefinery transformation strategies. Penetration of existing and mature value chains with replacement and substitution products, such as bio-fuels and added-value biochemicals, should be supported by adequate risk mitigation strategies against market uncertainties related especially to price fluctuation. Supply chain management strategies can provide control over product price volatility as well as the internalisation of market risks [3]. This paper examines the role of supply chain in the decision-making process for FBR business model definition based on the competitive assessment of a new product portfolio.

2. Value chain approach for product portfolio definition

Key drivers have been identified for the development of winning business models for the FBR [4] such as (1) the need to improve the variable and insufficient margins of the existing core business, (2) the need to transform the business model in place via the definition of a new product portfolio, (3) the need to secure future access to raw materials at a competitive price, and (4) the need to benefit from governmental. The new biorefinery product portfolio definition should respond to these drivers and lead to sustainable business profitability and growth [2]. In this regard, Porter [5] emphasizes that both *operational effectiveness* and *strategic positioning* are necessary but not sufficient for improving company's performance and creating profits.
Taking these elements into account, a systematic approach has been defined (Fig.1) considering market-driven as well as preliminary techno-economic-driven factors for product portfolio definition. A classical "design funnel" approach is used to define a set of promising product options, and then eliminate those that are less promising through market analyses, termed "evaluation of entry point" in existing or new value chains.

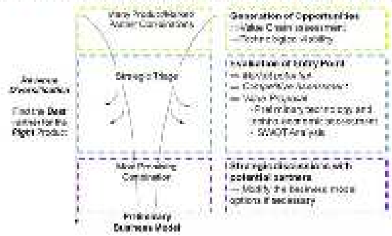

Figure 1.
Value Approach for Preliminary Business Model Definition

Market Potential Assessment

Bio-based replacement and/or substitution of existing products on the market requires a fundamental understanding of market dynamics, the potential for penetrating existing and mature value chains, and the related potential value proposals. Each product within a portfolio must be screened using a systematic assessment of its market potential taking into account a set of market, technology and techno-economic criteria such as market growth potential, product revenue potential, product yield potential to match market volume, margin creation, etc. The definition of the value chain point of entry is closely linked with the potential for partnering with a 'quality' third party [2]. As Hobbs observed [6], the value chain is a strategic network between a number of independent business organizations within a supply chain that share the goal of satisfying customers while sharing the risks and rewards of the chain.

Competitive Assessment

A major effort should be put on the competitive analysis of the overall portfolio in order to identify a unique value proposition for product delivery to a value chain, involving trade-offs that are unique to those of the competition [6]. For highly competitive markets such as the commodity market, product manufacturing and delivery cost-competitiveness are critical. On the other hand, for specialty products, differentiation and first-to-market strategies will drive the competitive advantage. From a *procurement perspective*, access to economically viable biomass constitutes a competitive advantage in the context of rising biomass costs and the significant biomass cost component of overall manufacturing costs. Fibre security via supply agreements on volume and price must support the market strategy and ensure a high level of EBITDA/t, i.e. potential of high margins for every tonne of purchased biomass. *From a process perspective*, a unique technology strategy, e.g. including process flexibility potential, should enable the adaptation of the product portfolio under changing market conditions. *From a marketing perspective*, the potential for product differentiation in price, quality or functionality and the potential for market penetration, i.e. relative market shares, drive the product portfolio positioning on the market. *From a sustainability perspective*, product portfolio competitiveness under market fluctuations in price and volume reflects the company's potential to control price volatility risks and maintain the EBITDA/t. *From a product delivery perspective*, the supply chain effectiveness and responsiveness represent a barrier to entry for the competition in terms of costs and uniqueness of the supply chain network [6]. All these competitive factors must positively impact the profitability of the product portfolio [5].

3. Implications of supply chain factors for product portfolio design

3.1. Product portfolio alternatives

Based on this approach, two example biorefinery product portfolios have been defined. In the first portfolio, Fischer-Tropsch liquids (FTL) are produced and separated to waxes and diesel. Then diesel is converted to jet fuel (JF). In the second portfolio, butanol, succinic acid (SA) and lactic acid (LA) are produced. The portfolios are summarized in figure 2.

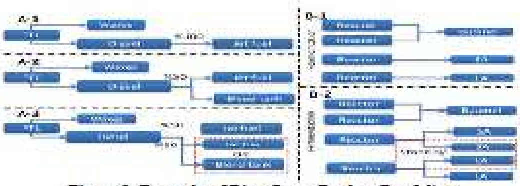

Figure 2. Example of Biorefinery Product Portfolios

3.2. Supply chain-driven factors for price volatility mitigation

Market price volatility is the result of supply issues as well as changes in global consumption, and demand due to economic factors and overcapacity [7]. For companies considering transformation to the biorefinery, this should be considered as a powerful opportunity for business model definition, and its impacts should be managed for gaining a potential competitive edge in both commodity and specialty markets (Fig.3). Responsiveness and effectiveness of the supply chain should be designed to respond to price movement systematically [8]. Key supply chain factors can help designing the product portfolio so that the market volatility risk is internalized.

Spot versus contracts

Considering that biorefinery product portfolios will be comprised of mixtures of commodity and specialty products, drivers for mitigating market volatility risks will be different from one product to the other. Commodity products are characterized by high volume and low margin markets (Fig.3), i.e. leading to low and often variable margin potential. Positioned upstream on the value chain and impacted by the variation of raw material costs, commodity prices tend to rise or fall with business cycles due to the lack of price control potential and the highly competitive environment [9]. Generally, specialty products have less volatility [9]. Specialty products, i.e. characterized by low volume and higher margins, are typically less exposed to changes in demand and prices, and lead to a more stable and higher EBITDA. Contract and spot sales strategies for both commodity and specialty products should take into account the potential for price control on the market, and benefits of price volatility mitigation on portfolio EBITDA.

Figure 3. Price volatility for different type of products

Manufacturing Flexibility and SC - Based on the example of product families A3 and B2 in Fig. 2, the potential offered by the process to switch from one manufacturing regime to another as defined at the process design stage is an important element for product portfolio competitiveness. Reactivity of the product portfolio offering enables the mitigation of the market volatility risks. The added capital and operating costs of this strategy may be compared to the gain in EBITDA on the product portfolio under different scenarios. Adaptation of the product portfolio offering towards more specialty products leads to the potential of benefiting from price control and maximizing the overall EBITDA/t along the portfolio.
Supply Chain Operating Strategy – The definition of the supply chain policy whose objective is supply chain profit maximization, should strategically consider both the choice of contract and spot strategy, and the manufacturing flexibility strategy, i.e. the potential for exploiting manufacturing flexibility [10]. As a critical element for designing and managing a competitive product portfolio, the supply chain policy should be part of the value proposal assessment of each product portfolio, representing the potential for margins improvement for the overall product portfolio.

4. Conclusions

The unique supply chain strategy, combining procurement and product delivery strategies, is a critical decision-making factor for designing biorefinery product portfolios, and a necessary tool for internalizing market volatility factors. A key indicator in the potential of the supply chain strategy at the product portfolio level is the EBITDA/t. This work was supported by Natural Sciences Engineering Research Council of Canada (NSERC) Environmental Design Engineering Chair at Ecole Polytechnique in Montréal.

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APPENDIX I – Book Chapter: Forest biorefinery supply chain design and process flexibility

Forest Biorefinery Supply Chain Design and Process Flexibility

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Summary

For a forestry company to improve its business model in the current market situation, it not only should diversify its revenue, but also must change its current manufacturing culture, i.e. focusing on capacity management and neglecting SC profitability. This manufacturing culture will be changed, in the short term, by applying novel SC operating policies which help to reduce SC costs and maximize SC profit by exploiting production flexibility, and in the long term, by using advanced decision-making tools.

The goal of this chapter is to show how an SC-based analysis enables decision-makers to analyze various biorefinery options systematically from an SC perspective on biorefinery (BR) strategic design and to evaluate them under different market conditions based on the impacts of the design of each option on tactical-operational activities. A hierarchical methodology is developed to integrate flexibility design and SC network design, while accounting for operational-level activities at the design level.

This chapter is organized as follows. First, the key concepts used in this approach, i.e. margins-based SC operating policy, manufacturing flexibility, and the bottom-up approach, are introduced. Then, flexibility, which is the major focus of this chapter, is reviewed, various flexibility definitions, problems, and types are introduced, and the meaning of flexibility in the BR context and product-process considerations for a flexible BR option is discussed. Later, the SC optimization framework and how it is used in the margins-based approach are discussed. Finally, the proposed methodology for SC-based analysis is presented, along with an illustrative example to highlight the importance of implementing the proposed methodology.

Book chapter in *Integrated Biorefineries: Design, Analysis, and Optimization*

The contribution of this chapter is:

- To create a more concrete definition of the margins-based concept in SC optimization and to reflect the effect of tactical-operational-level activities at the design level by means of a margins-based policy;
- To incorporate SC considerations into the determination of process operating windows by using margins-based SC optimization along with techno-economic studies;
- To apply a scenario-based approach to designing the SC network to provide a better reflection of the practical aspects of redesigning the SC at the decision-making level.

1. Introduction

For a forestry company to improve its business model in the current market situation, it not only should diversify its revenue, but also must change its current manufacturing culture, in which the management focus is on capacity management and the profitability of the entire supply chain (SC) is generally ignored.

According to the strategic phased approach for the forest biorefinery (FBR), revenue diversification will be achieved by means of "technology disruption" by producing building-block biorefinery chemicals, and ideally, in the longer term, by further increasing revenues by producing added-value derivatives. On the other side, manufacturing culture will be changed, in the short term, via "business disruption," through applying novel SC operating policies and exploiting production flexibility, and in the long term, by using advanced ERP and decision-making tools.

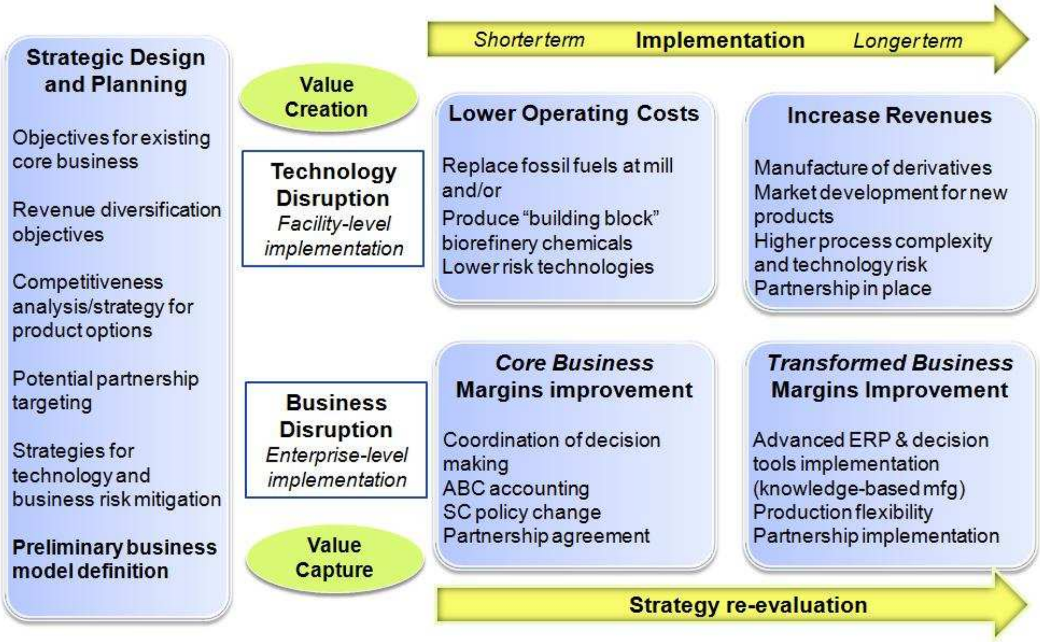

Figure 1. Strategic implementation of the biorefinery by a P&P company.

The key to success for "business disruption" is SC analysis. In the short term, to mitigate the risks of market volatility, companies should focus on improving their margins by implementing a *margins-based SC operating policy* and better exploiting the process capability for *flexible production* by using detailed knowledge of the process and its cost structure. Then advanced SC optimization techniques can be used to carry out product planning over different time horizons and to identify tradeoffs between product orders and anticipated supply and demand. This approach shows the importance of advanced cost-accounting systems that are capable of reflecting the cost of each decision at the decision-making level for short-term decision-making activities. Over the long term, companies should base their strategic SC-related decisions on a bottom-up approach, i.e. designing/redesigning the SC based on the impact of the design on tactical and operational activities. These two approaches to the short-term and long-term aspects of biorefinery implementation, the margins-based approach and the bottom-up approach, imply profound changes in the way forestry companies do business today, which is equivalent to business disruption.

The goal of this chapter is to show how SC-based analysis enables decision-makers to analyze various biorefinery options systematically from an SC perspective on biorefinery strategic design. These biorefinery options will be identified by the company's experts based on their experience and knowledge of the company, future forecasts, the assets of the company's existing

SC, the potentials of the company's SC for biorefinery implementation given the latest developments in biorefinery technologies, and eventually the SC potential for forming partnerships with other companies. The SC-based analysis developed here analyzes these options and reveals the value that would be unleashed by the realization of each. This chapter is the evolution of the authors' recent paper published in *Computers & Chemical Engineering*, entitled "Integrating product portfolio design and supply chain design for the forest biorefinery" [1]. The methodology presented in this chapter is a modified version of the methodology proposed in this paper, with more emphasis on the design aspects of the SC, i.e. flexibility design and SC network design. The specific contributions of the paper and the chapter are illustrated in Figure 1.

	Main objective and sub-objectives of the paper	Main objective and sub-objectives of the chapter
Title	**Integrating product portfolio design and SC design for the forest biorefinery**	**Forest biorefinery SC design and process flexibility**
Objective	To develop a hierarchical methodology to integrate market, technical and SC analysis to determine the best set of products to be produced in a biorefinery	To develop a hierarchical methodology for biorefinery strategic SC design that integrates the manufacturing flexibility design with SC network design
Sub-objective	To introduce a set of market criteria to define product portfolio To introduce large block analysis to define process portfolio To define product/process portfolio	To concretize the margins-based concept in SC optimization To reflect the effect of tactical-operational level activities at the design level via the Margins-based SC policy
	To establish a design target for a flexible process system To design the established design target Margins-based SC optimization plays the key role in both steps	To incorporate SC considerations in determining the operating window of processes by utilizing margins-based SC optimization along with techno-economic studies
	To design the SC network based on its effect on tactical and operational level activities	To apply a scenario-based approach in designing the SC network to better reflect the practical aspects of redesigning the SC at the decision making level

Figure 1. Comparison between title, main objective, and subobjectives of the chapter and the *Computers & Chemical Engineering* paper

At this point, the key concepts used in the chapter, margins-based SC operating policy, manufacturing flexibility, and the bottom-up approach are introduced. These concepts play key roles in the methodology, and in light of them, the goals of the methodology can be better understood.

1.1. Margins-based operating policy

The operating policy in the P&P industry is said to be "manufacturing-centric." In this industrial sector, the management focus is on capacity planning, and industry participants try to achieve the efficient and effective use of machine capacity [2]. As a result, process efficiency is viewed as the key measure for profitability, and therefore it is believed that minimizing production cost will result in the highest profitability [3]. Moreover, production planning assumes a known set of orders and a fixed sequence of product grades. By treating the manufacturing process as the focal point, inventory and changeover costs are typically ignored or considered separately [2], and SC costs are often neglected, resulting in lower profitability [3].

To implement the FBR, the operating policy must shift from a manufacturing-centric approach to a margins-based one. This latter operating policy tries to maximize margins over the entire SC and to produce and select products and orders that ensure the best returns [3]. In this approach, long-term contracts and short-term order selection is made with respect, not only to process and production constraints, but to all SC constraints, including for example inventory and transportation constraints, to maximize the ultimate SC profitability.

1.2. Manufacturing flexibility

Today's market is subject to huge volatilities in terms of price and demand. The price of oil, fuels, and chemicals, as well as the price of forestry products, change even on a monthly basis. The demand for some products is not always certain, and sometimes, despite strong demand, the price is too low for the production of a product to be profitable. On the feedstock side, uncertainty exists in terms of price and availability. A forestry company might be obliged to procure its feedstock from different sources over different distances and with different prices. Short product life cycles and increasing competition among companies reveal new uncertainties and risks for different industries. Specialty chemicals impose additional financial risks and uncertainties because customers are granted a very high degree of flexibility in terms of demand quantity. A reveal date is assigned to each product at which the customer specifies his final demand. Some companies even give their customers the right to cancel and withdraw the order at this point [4]. All these clauses entail more uncertainty and risk for the companies. To mitigate risks in the face of such uncertainties, it is of crucial importance to enhance adaptiveness and reactivity on one hand and proactivity on the other hand [4]. These capabilities are generally called *flexibility*. Based on the type of uncertainty and how it is addressed, there are different types of flexibility, which will be discussed later in this chapter.

An FBR would be exposed to this kind of volatile environment and would face these risks and uncertainties. Hence, flexibility, of any possible type, must be exploited in a FBR to mitigate risks. An FBR will be able to produce several products, including P&P products, bioproducts, and energy. Producing several products implies the opportunity to take advantage of manufacturing flexibility, i.e., producing different products at different volumes in different time periods. In a volatile market, depending on feedstock and product prices as well as supply and demand, manufacturing flexibility can be exploited, and the mill can produce different products in different amounts to optimize and secure the company's margin. The company should analyze its access to feedstocks, product prices, and received as well as forecasted demands and find the best alignment between these demands and its production capacity to maximize the company's profit.

1.3. Bottom-up approach

As mentioned in the definition of the margins-based policy, the ultimate goal of this policy is to maximize profitability across the entire SC. In fact, the margins-based operating policy exploits the manufacturing system's capability for flexible production at the SC operational level to maximize the margins. Therefore, an SC-based analysis is needed to show how the flexibility capability should be managed and exploited at the SC operational level to maximize SC profit. At the design level, flexibility must be designed in a way that ensures the best performance at the operational level and the attainment of the ultimate goal, i.e., maximizing the SC profit. Hence, there should be a metric representing SC profitability that can reflect it at the design stage. Moreover, from a SC design perspective, the SC network must be designed so that it enables margins-based operating policy to exploit flexibility. In other words, the SC network should be designed in such a way that it serves the maximum exploitation of flexibility for profit maximization. Therefore, an SC-based analysis is required to address both aspects: operational and design. Hence, the challenge is to develop a SC-based analysis which can be used:

- At the design stage, to reflect SC profitability as a design metric in the flexibility and SC network designs;
- At the tactical-operational level, to improve SC profitability by exploiting flexibility.

Figure 2 provides a schematic illustration of the linkage between SC analysis and design and operational decisions.

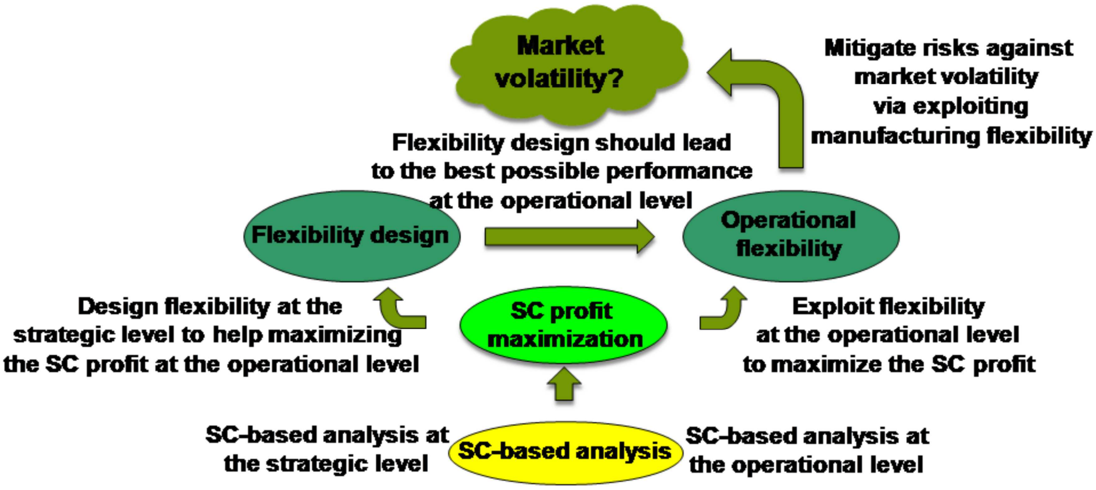

Figure 2. Linkage between SC-based analysis and design/operational decisions.

The bottom-up approach shows the importance of operational-level information for design-related decisions and implies that such information should be brought up to the strategic-level decision-making to obtain a system with greater flexibility in its performance.

To address the linkage between designing a flexible manufacturing system and designing its associated SC, considering the impacts of such decisions on tactical-operational SC activities, this chapter introduces a methodology which involves an SC-based analysis as the focal point. The proposed methodology incorporates SC management into designing a flexible manufacturing system using the margins-based operating policy.

The rest of the chapter is organized as follows. First, flexibility as the major focus of this chapter is reviewed. Next, the SC optimization framework and how it is used in the margins-based approach are discussed. Afterwards, the proposed methodology for SC-based analysis is presented. Each step of the methodology is described, and the way that SC modeling is used in each step is explained. An illustrative example is presented along with the methodology to highlight the importance of implementing the proposed methodology.

2. Biorefinery process flexibility: definition, importance, problems, and types

In this section, different definitions of flexibility and its importance are discussed. Then, the problems identified and studied to date related to flexibility are presented, and different types of flexibility are introduced. Finally, a concrete definition is provided of the concept of flexibility which forms the basis of the methodology presented here.

2.1. Definition

One of the earliest definitions of manufacturing flexibility goes back to Ropohl (1967), who considered manufacturing flexibility as “the property of the system elements that are integrally designed and linked to each other in order to allow the adaptation of production equipments to various production tasks” [5]. Another early definition of flexibility was proposed by Gupta and Goyal (1989), who defined it as “the ability of a manufacturing system to cope with changing circumstances or instability caused by the environment” [6]. From an operational point of view, Nagarur (1992) defined flexibility as “the ability of the system to quickly adjust to any change in relevant factors like product, process, loads and machine failure” [7]. Upton (1994) provided a more comprehensive definition which addressed flexibility as “the ability to change or react with little penalty in time, effort, cost or performance” [8]. Sethi and Sethi (1990) did a comprehensive survey on the concept, reviewing different definitions and types of manufacturing flexibility. They defined the flexibility of a system as its adaptability to a wide range of possible environments that it may encounter. In other words, a flexible system must be capable of changing to deal with a changing environment [9]. In the chemical engineering context, Grossmann et al. (1983) defined flexibility as the ability of a manufacturing system to satisfy specifications and constraints despite variations that may occur in parameter values during operation [10].

From a hierarchical decision-making point of view, flexibility can be classified as long-term (strategic), midterm (tactical), and short-term (operational) flexibility. These levels can be defined respectively as: (i) the ability of a system to respond to changes in strategy, new product introductions, and basic design changes, (ii) the ability to operate at varying rates, to accept random, minor changes, and to convert the plant for alternative uses, and (iii) the ability to reset and readjust between known production tasks to permit a high degree of variation in sequencing and scheduling [11].

Several reasons have been mentioned for the importance of flexibility. Frazelle [12] believed that flexibility is required to maintain competitiveness in a changing business environment of which the critical features are rapidly decreasing product half-life, the influx of competitors, an increasing demand for product changes, and the introduction of new products, materials, and processes. Slack (1983) saw the incentives for flexibility in the instability and unpredictability of the manufacturers' operational environment and in developments in production technology [13].

2.2. Flexibility problems

From a broad perspective, flexibility problem areas can be categorized into two groups: flexibility design and flexibility analysis.

2.2.1. Flexibility design

In this type of problem, the design is unknown, and the problem is to find the optimal design of a system considering the costs incurred by that design. A design representing a higher degree of flexibility will have a lower probability of encountering an infeasible operating condition, but at a higher cost. Two major areas have been considered by Grossmann et al. (1983): optimal design with a fixed degree of flexibility, and design with an optimal degree of flexibility [10].

2.2.1.1. Optimal design with a fixed degree of flexibility

The flexibility of a design is optimal when the economic advantages of flexibility are balanced in relation to its cost. In this problem, a design should be identified that can operate over varying conditions. These varying conditions must be specified as a bounded range of parameter values over which the design is able to meet the specifications at minimum cost. In this type of problems the required degree of flexibility has already been specified, either by a discrete set of required operating conditions, or by requiring feasibility of operation when a set of uncertain parameters varies between fixed bounds. Therefore, this class of problem can be divided into two categories [10]:

c) Deterministic problems, or problems of deterministic multiperiod design, in which the plant is designed to operate optimally under various conditions over a sequence of time periods. The goal is to ensure that the plant will be able to meet the specifications over successive periods of operation.

d) Stochastic problems, or problems of design under uncertainty, which address the design of chemical plants under conditions where the values of some of the process parameters have significant uncertainty. However, a particular design problem as presented might include both these problems.

The ultimate goal in solving these types of problems is to ensure that the design, while being economic, meets the specifications under different imposed conditions.

2.2.1.2. Design with optimal degree of flexibility

In this type of problem, the desired degree of flexibility is not known, and a design with the optimal degree of flexibility must be identified. The optimal degree of flexibility does not necessarily imply the highest degree of flexibility, because another criterion, which is the cost of the design, is important in determining optimality of a design. In fact, design with optimal degree of flexibility addresses problems which needs establishing a tradeoff between the cost of the plant and its flexibility. Therefore, the objective function can be separated into two components: minimizing capital and operating costs on the one hand, and maximizing flexibility on the other hand. The result will be a tradeoff curve which relates flexibility and cost. Hence, the major task in this type of problem is to determine the degree of flexibility. In other words, a metric or a quantitative measure of flexibility in the form of a scalar index is needed that can measure the size of the region of feasible operation for the design. This metric is called the *flexibility index*. Flexibility-index problems involve designing the plant with the aim of both cost minimization and flexibility-measure maximization. Problems in this category have evolved from flexibility-index problems [14] to stochastic flexibility-index problems [15] and expected stochastic flexibility-index problems [16].

2.2.2. Flexibility analysis

In flexibility analysis problems, the design of the plant is given, and the goal is to analyze the plant's capability for feasible operation. Two types of problems can be defined in this category;

2.2.1.3. Feasibility or flexibility test

In this type of problem, it is determined whether the design can operate feasibly at all uncertain points in the range. More specifically, the objective of the feasibility problem is to determine whether, for a given design, set of nominal values for the uncertain parameters, set of expected deviations in the positive and negative directions, and set of constraints, at least one set of control variables can be chosen during plant operation such that, for every possible realization of the uncertain parameters, all the constraints are satisfied [17]. Halemane and Grossmann (1983) carried out one of the earliest studiesworks in this domain and showed how, for a given design and a fixed parameter value, the max-min-max problem provides a measure of the size of the feasible operating region [18]. Grossmann and Floudas (1987) presented mathematical formulations for the feasibility test based on the property that the number of active or limiting constraints on flexibility is equal to the number of control variables plus one, provided there is linear independence among the active constraints [19]. Bansal et al. (2000) introduced a unified theory and algorithms based on multiparametric programming techniques for the solution of feasibility test problems in linear process systems [20]. Floudas et al. (2001) presented an approach for feasibility test problems based on the principles of the αBB deterministic global optimization algorithm, which relies on a difference-of-convex-functions transformation and a branch-and-bound framework [21]. Goyal and Ierapetritou (2003) developed an algorithm for evaluating the feasibility of nonconvex processes, based on the idea of systematically determining the infeasible areas using an outer approximation procedure and a simplex approximation approach to approximate the expanded feasible space which can be constructed by the exclusion of nonconvex constraints [22].

2.2.1.4. Flexibility index

The aim of flexibility-index problems is to determine how flexible a given design is. In other words, the maximum deviation that the design parameters can tolerate must be determined. The major issue in these problems is to define a quantitative measure for the degree of flexibility. A scalar metric, called the index of flexibility or the flexibility index, can be developed, for which the value characterizes the size of the region of feasible operation in the uncertain parameter space. In other words, it can be defined as the largest-scale deviation of any of the expected deviations that the design can handle and still operate feasibly [14].

Grossmann and Floudas (1987) addressed the analysis of the flexibility of a proposed design using an active constraint strategy and MINLP formulations for flexibility-index problems [19]. Pistikopoulos and Grossmann (1988) worked on redesigning existing process flowsheets to increase their flexibility. The major difficulty in such retrofit problems is that of deciding which parameter or structural changes are required, with the aim of increasing flexibility at the least investment cost. Their proposed approach for the retrofit design problem involves: (a) a systematic procedure for handling parametric changes of the design variables, (b) embedding a strategy for handling simultaneous structural and parametric changes, and (c) a procedure for developing tradeoff curves between cost and flexibility [23]. Bansal et al. (2000) presented algorithms based on multiparametric programming techniques for the solution of flexibility analysis and design optimization problems in linear process systems which are used to solve flexibility-index problems in systems with deterministic parameters. The algorithms as developed are computationally efficient and reveal explicitly the dependence of various flexibility metrics on the values of the continuous design variables [20].

2.3. Flexibility types

Many efforts have been made to categorize various types of flexibility. The common element in all types of flexibility is that they are used to mitigate the risks associated with different types of uncertainty. These uncertainties are the results of variations in the temperature, pressure, or flowrate of a stream, changes in the state of equipment, or fluctuations in the price and demand of products. Based on the type of uncertainty, specific types of flexibility can be defined. Sethi and Sethi (1990) introduced 50 different terms for different types of flexibility, although their definitions were not always precise and, for identical terms, not always in agreement with one another [9]. Swamidass (1988) pointed out the difficulties of understanding and therefore categorizing flexibility to be (i) the use of flexibility terms with overlapping scopes, (ii) the use of flexibility terms with different meanings and (iii) the use of flexibility terms which are aggregates of others [24]. Beach et al. [11] carried out a comprehensive survey on the concept and types of flexibility and concluded that the original eight categories of flexibility defined by Browne et al. (1984) [25] represent the most comprehensive classification of flexibility. They classified manufacturing flexibility in a discrete manufacturing environment into eight categories: machine, process, product, routing, volume, expansion, operation, and production.

In the chemical engineering context, four major types of flexibility have been widely studied widely: recipe, product, volume and process. The definition of each flexibility type is given in Table 1.

Table 1. Types of flexibility and their definition.

Flexibility	Definition
Recipe	The ability to have a set of adaptable recipes that can control the process output
Product	The ability to change over to produce a new (set of) product(s) economically
Volume	The ability to operate a system profitably at different production volumes
Process	Capability of the process to operate feasibly under changing conditions

2.3.1. Recipe flexibility

The flexible recipe concept was originally introduced as a set of adaptable recipes that can control the process output and can be modified to confront any deviation from nominal conditions. Recipes specify products and prescribe how products are to be produced. The nominal recipe for a given product represents the optimal compromise between quality and costs. According to the production scenario, recipes can be changed or modified. Verwater-Lukszo developed this basic idea and introduced the concept of the flexible recipe as a way of systematically adjusting control recipes during the execution of production tasks with the aim to enable the process to perform under different operating conditions [26]. These changing operating conditions may include different feedstock properties, changes in quality specifications, variations in process behavior, new market conditions, other real-world experiences with the process, and so on, none of which is reflected in the recipes, although it would often be profitable to be able to adapt them to the changed conditions.

One of the first attempts to do so was made by Romero et al., who extended the flexible recipe approach to a plant-wide scheduling problem [27]. Another study was carried out by Ferrer-Nadal et al., who aimed to optimize production scheduling in a batch plant where flexible recipes were used. They integrated a linear flexible recipe model into a multipurpose batch-process scheduling formulation, which in turn, enabled integration between a recipe optimization procedure at the control level and a batch-plant optimization strategy [28]. Laflamme-Mayer et al. (2008) developed an SC planning model that exploits the capability of a market pulp mill to use different recipes in a flexible manner to provide adequate support for cost-effective fiber supply use [29].

2.3.2. Product/Volume flexibility

Product flexibility, according to Browne et al. (1984) [25], is the ability to change over to produce a new product economically and quickly. This definition is consistent with the concept introduced by Sahinidis and Grossmann (1991) [30] and referred to as *flexible production*, which addresses the capability of a manufacturing system to produce different products at different times (different production modes). This type of flexibility is generally used in conjunction with volume flexibility, which is the capability of a facility to operate at different production rates. Examples of such flexible facilities include pulp and paper mills which can produce different grades of pulp and paper, or refineries that process different types of crude oil at different volumes [31]. According to Sahinidis and Grossmann [30], a flexible process network consists of dedicated and flexible production facilities that can be interconnected in an arbitrary manner. Dedicated production facilities manufacture fixed amounts of a set of high-volume products at all times, while flexible production facilities, which are normally used for producing low-volume products, manufacture different products at different times.

One of the first studies in this context was carried out by Sahinidis and Grossmann [30]. They addressed a network of existing and potential processes and chemicals. The processes can be dedicated or flexible, continuous or batch. Given a forecast of prices and demands, as well as investment and operating costs over a specific time horizon, the objective is to determine capacity expansion and shutdown policy for existing processes, selection of new processes and their capacity expansion policy, production profiles, and sales and purchases of chemicals at each time period. The objective function is the net present value which must be maximized. This work was continued by Norton and Grossmann, who considered flexibility in raw materials [32]. In this study, processes with potential flexibility on either the feedstock or the product side, as well as processes with flexibility on both sides, are considered. These two studies were dedicated to long-term planning problems. In a more recent study, Bok et al. addressed detailed operational decisions in continuous flexible process networks. The model presented in this study extends previous models by incorporating an inventory profile, changeover costs, intermittent supplies, and production shortfalls [31]. As mentioned earlier, this approach is widely used in refineries and the petrochemical industry. Petrochemical complexes are able to produce several products by means of processes which can operate over a range of production rates. Neiro and Pinto (2004) [33] and Schulz et al. (2005) [34] described SC planning in petrochemical complexes which use this strategy. Mendez et al. (2006) explained the scheduling of oil-refinery operations, in which continuous processes produce a set of components at constant flowrates and then a blending process is used to transform these components into different derivatives in varying amounts.

2.3.3. Process flexibility

In the chemical engineering context, process flexibility has gained the most attention. From a general point of view, process flexibility is a property of *process operability*. Grossmann et al.

(1983) break down operability into a set of properties such as flexibility, controllability, reliability, and safety [10]. Flexibility is concerned with the problem of ensuring feasible operation of a plant over a whole range of conditions in both steady-state and dynamic environments, while controllability signifies the ability of a plant to move efficiently from one operating point to another as well as to deal efficiently with disturbances [36]. Reliability denotes the capability of the process to withstand mechanical and electrical failures, and safety is the prevention of major hazards given possible failures.

Grossmann et al. (1983) mentioned the need for accounting operability considerations, mainly related to flexibility and controllability, at the design stage [10]. Blanco and Bandoni (2003) named three major approaches to the design-for-operability problem [37]:

- Heuristics

Heuristics rely on rules of thumb. Such recipes can be found in Douglas's famous book on conceptual design [38].

- Operability measures

Operability measures have been widely used in both open-loop and closed-loop controllability. They describe specific operability features and are used to screen or classify different designs with respect to a particular operability issue. Controllability and resiliency indices such as RGA, NI, DCLI, and SVD are examples of these indices [37].

- Complete integration

This approach implies the integration between process design and process operability by including operability elements within the process design formulation. This approach takes advantage of multiobjective optimization and can be seen in the works of Grossmann and Pistikopoulos [14]. Heat exchanger networks have been used as a classical example in such studies. Hot and cold process streams are considered as uncertain parameters and, given the nominal values of the temperatures and the flowrates and assuming expected deviations of the temperatures, e.g. ± 10°K, the goal is to determine whether the network can tolerate changes in inlet temperatures over the specified range [19]. Pistikopoulos and Grossmann (1988) addressed a stochastic flexibility problem in which the major issue is to determine the appropriate tradeoff between the investment cost for the retrofit design of a system and the expected revenue that will result from having increased flexibility [23]. For this purpose, a number of redesign alternatives with specified degrees of flexibility were obtained from a tradeoff curve which related retrofit cost to flexibility. Then, for these designs, the corresponding expected optimal revenue was evaluated using a modified Cartesian integration method. Pistikopoulos and Grossmann (1989) extended this work for nonlinear models [39].

2.3.4. Manufacturing flexibility in the FBR

The concept of manufacturing flexibility in the FBR implies the ability to produce several bioproducts at different volumes, i.e., different production rates, in different time periods based on product price and demand. From an economic-market perspective, this type of manufacturing flexibility implies a justifiable increase in capital cost that is adequately compensated by the ability of the process to manufacture in a flexible manner so that the expected volatility in market conditions can be mitigated. The proposed definition seems to be an aggregation of product flexibility and volume flexibility. Because process flexibility is inherent in the design of each chemical process, this definition has already included process flexibility. Finally, experts believe that feedstock flexibility is a promising element in the success of the FBR. BR processes, especially thermochemical processes, can accept a wide range of feedstocks. This makes it possible to keep operations running with different types of feedstock and to have the flexibility of procuring feedstock from different sources. It will also be a competitive advantage for the company in the volatile feedstock market, where it must deal with several considerations such as feedstock price, competition from other businesses, sufficient availability, handling, proximity, seasonality, and collection. Therefore, feedstock flexibility is another dimension that must be addressed in the definition. Hence, the definition of manufacturing flexibility in the FBR can be interpreted as the aggregation of feedstock, process, product, and volume flexibility, with volume and product flexibility as the major dimensions.

The FBR presents a promising opportunity to implement manufacturing flexibility as defined here. The FBR processes are retrofit to P&P mills which are in place with a known level of flexibility. The FBR and P&P mills might be integrated in terms of feedstock, chemicals, and energy. Hence, the P&P process flexibility can be characterized first, and then the BR process and its flexibility can be designed based on the flexibility of the P&P side, as well as product price and demand. This will provide the opportunity to produce both P&P products and bioproducts, which will improve P&P companies' business model and might prevent current mill closures [40]. This strategy was used successfully in previous decades, when forestry companies were producing ethanol as a side product as well as forestry products as main products. In today's market, where the demand for P&P products is decreasing for several reasons such as the presence of global low-cost producers, this strategy can be pursued in another way, by shifting the core business from a forest-products producer to a bioproducts producer that also produces forestry products.

In the FBR context, there are two strategies with regard to the products that can be produced: large-scale commodity production, and commodity/specialty or low-value/high-value commodity production. The commodity chemicals considered in the first strategy are mainly limited to ethanol and butanol because these can be used as fuel. The idea that supports this strategy is that there is a huge market for such commodities in the fuel market, especially in the United States. However, another strategy has been gaining attention: production of specialty chemicals or a combination of small-volume value-added products and large-volume low-margin products [41,42,43]. Fine and specialty chemicals are said to be promising elements of an FBR product portfolio because they have bigger margins than P&P products a better market with less competition, so that the FBR does not have to compete with huge well-established commodity petrochemical products. Because fine and specialty products are produced in smaller volumes, they need less feedstock. This is a competitive advantage for a production environment like a biorefinery for which procuring biomass as feedstock is a great challenge.

A study has been done by the National Renewable Energy Laboratory (NREL) [43] on the analysis of biorefineries, in which the importance of coproducing high-margin low-volume products along with a primary product is addressed. The advantages of such a product portfolio compared to dedicated production of a single product can be classified into two levels: long-term and short-term. The long-term advantages are summarized as follows:

- Product diversity mitigates risks associated with seasonal demand cycles and market downturns.
- If selected coproducts have the potential to become platform intermediates in future, their commoditization will be fostered by taking advantage of the economies of scale provided by producing small amounts of the coproduct in a commodity-producing biorefinery. An

ethanol plant producing succinic acid, lactic acid, and/or butanol as coproducts is an example. As mentioned in the NREL report, early-generation ethanol biorefineries can serve as incubators for chemicals that can then become high-volume products in their own right.

The short-term advantages are as follows:

- Revenues from high-value coproducts reduce the selling price of the primary product.
- The economies of scale provided by a full-size biomass refinery lower the processing costs of low-volume, high-value coproducts.
- Less fractional market displacement is required for cost-effective production of high-value coproducts as a result of the economies of scale provided by the primary product.
- Biomass refineries maximize the value generated from heterogeneous feedstock, making use of component fractions.
- Common process elements are involved in producing fermentable carbohydrates, regardless of whether one or more products are produced.
- Coproduction can provide process integration benefits (e.g., meeting process energy requirements with electricity and steam cogenerated from process residues).

For such a plant to be competitive with other commodity producers, a very important point in this strategy is to be able to produce such commodities in large volumes. Commodity buyers prefer to buy the products they need from a single seller so that they can negotiate with the product provider on price and so that they can avoid buying from several sellers to reduce their transportation costs. Therefore, it is important for a producer to be able to produce commodity products in large volumes so that it can respond to large customers. This underlines the importance of feedstock procurement for the company.

2.3.5. Process considerations for a flexible biorefinery option

From a generic point of view, chemical processes can be classified into two major categories, continuous and batch. Continuous processes are appropriate for large-scale production lines because they are designed to operate 24 hours a day, seven days a week over the whole year at almost constant conditions. The plant is shut down only for maintenance or in emergency situations. On the other hand, batch processes are designed to be started and stopped frequently because during operation, units are filled with materials, perform their function, and are then stopped, drained, and cleaned to be ready for another cycle [38].

There are certain guidelines for when a batch process may be chosen over a continuous process [38];

- Production rate or capacity: Plants with capacity of greater than 10×10^6 lb/yr are usually continuous, while plants having a capacity less than that are normally batch.
- Market forces: Batch processes are more flexible in terms of both throughput and number of products. In fact, a large number of products can be produced in the same production line. As a result, batch processes are used to manufacture products that have seasonal demand.
- Operational problems: Some processes involve slow reactions, slurries with settling solids, or materials that foul the equipment rapidly. In these cases, batch processing is an ideal option, because it gives the process the time it needs, and the processing units can be stopped and cleaned after any operation involving settling or fouling materials.

Based on these characteristics of batch and continuous processes, if the desired strategy is to produce commodity chemicals, then a continuous process should be chosen because the production volume must be large enough to enable the company to enter the commodity market. However, it must be remembered that continuous processes have limited potential for flexibility because they are dedicated to one or a few products and their throughput is to some extent fixed. Moreover, commodity production does not have large margins needs huge amounts of biomass as feedstock.

If the desired strategy is to produce value-added products, batch processes should be chosen. Fine and specialty chemicals are produced in batch systems. Being able to respond appropriately to market changes is of great importance in today’s market, and as explained earlier, flexible batch processes enable companies to produce different products in different volumes at different time periods. Therefore, based on product price and demand, production can be scheduled in such a way that in every time period, be it a week, a month, or a season, the most profitable products are produced in the right volume. Batch processes will become more important as the dedicated nature of continuous processes is addressed. Continuous processes are generally designed to produce one specific product. Therefore, even if the production rate of a continuous process is decreased to produce only the amount needed to fulfill the profitable orders, the excess capacity cannot be used to produce another product. This will have an enormous impact on the rate on return on investment. However, a batch system can be changed over to produce a more profitable product, and the whole capacity of the system can always be used.

3. SC optimization with margins-based operating policy

As discussed in the introductory section, flexibility should be exploited at the operational level to maximize SC profit. Because the margins-based approach is to be used as the operating policy of the biorefinery production facility, flexibility must be exploited using the margins-based approach to maximize SC profit. Hence, an SC-based analysis must be used to reflect this approach at the SC tactical operational levels. On the other hand, according to the bottom-up approach, SC profitability must be reflected as a design metric at the strategic decision-making level, and therefore, once again, the necessity of an SC-based analysis becomes apparent. Such an analysis will use an SC optimization framework which will consider feedstock price and availability, production costs, and inventory and delivery costs, as well as product price and demand. Taking this information and these constraints into account, the SC optimization framework will exploit the potential for production flexibility and determine which orders must be fulfilled and therefore how much of which products must be produced, how they should be stored, and how they should be delivered to the market to maximize SC profit.

The focus of this chapter is on the role of SC analysis in the design problem. Therefore, in the next section, the SC framework will be explained, and in the following section, its function in a design problem will be discussed.

3.1. SC framework

The SC framework aims to maximize profitability across the entire SC by first identifying the tradeoffs between demand and production capabilities and then by finding the optimal alignment of manufacturing capacity and market demand. The SC framework is formulated as an optimization problem with the objective of maximizing profit. This framework considers the management of a multi-product, multi-echelon SC, including existing production, warehousing, and distribution facilities as well as a number of customer zones, although it can also be used for design purposes, as will be discussed in Section 4. Production facilities can make one or several products. Warehouses can receive material, either feedstock or product, from different sources and plants and supply different distribution centers, while distribution centers can supply different markets. Each market places demand in two ways: by contract, i.e., for the long term, and in the spot market, i.e., for the short term. The optimization problem is formulated into an MILP (mixed-integer linear program). Like every optimization problem, the SC framework consists of an objective function, decision variables, constraints, and parameters. In the following parts of this chapter, these components of the SC framework are explained.

3.1.1. Decision variables

There are two types of decision variables in the mathematical formulation of the SC. The first type is continuous variables, which represent variables that can take on continuous values. They describe the flow of material between SC nodes, e.g., the flow of feedstock from suppliers to the mill, production rates for each product showing the amount of each product to be produced, rates of product flow from plants to warehouses, to distribution centers, and to markets, and inventory levels for each type of feedstock and product. In a design problem, where the capacity of the facilities, e.g., the production capacity, is unknown, a decision variable is assigned to the unknown capacities. Therefore, based on the goal of the design problem, the capacities of plants, warehouses, and distribution centers can be represented by continuous decision variables [44].

The second type of decision variable is binary variables which imply a “yes/no” type of decision, e.g., which order should be taken, which product must be produced, which production line must operate, which warehouse should supply which distribution center, and which distribution center should supply which market. In a strategic design problem, decisions such as which product to produce and which market to supply for the long term, which location to choose for a facility, and which partner to incorporate with, can be represented by binary variables [44]. However, because the number of binary design variables is usually small, such decisions can also be made using a scenario-based approach, i.e., generating a scenario for each design option. This approach is used in the methodology presented in this chapter and will be discussed in more detail later.

3.1.2. Constraints

Each node of the SC, such as suppliers, inventories, and manufacturing centers, has its own constraints which must be formulated mathematically. They can be classified as follows [44]:

- Network structure constraints determine which nodes of the SC can be linked to each other and whether material can flow between them.
- Material balance constraints relate the flow of material into and out of different SC nodes to the accumulation, production, and consumption of material in that node.
- Capacity constraints represent the minimum or maximum amount of material that can be produced or stored in a node. Production capacity is generally modeled as a linear constraint which relates the production rate of a product to the availability of feedstock. The capacities of warehouses and distribution centers are described by upper and lower bounds on their material-handling capability.
- Nonnegativity constraints ensure that all variables are greater than zero.

3.1.3. Objective function

The objective function can be defined in two ways;

- Operating costs: Operating costs include the costs incurred in feedstock procurement and material production at plants, as well as transition and shutdown costs, material handling at warehouses and distribution centers, and transportation of material throughout the entire SC. These costs are calculated on a daily basis. If the objective function were calculated in terms of the operating cost, the goal would be to minimize the objective function. In SC design problems, the objective function can be defined as the sum of operating costs and capital costs. The capital costs are the costs associated with the establishment of the SC infrastructure, calculated on a long-term basis.
- Profit: Profit is the sum of revenues from different main products and byproducts minus the operating costs. In this case, the goal is to maximize the objective function. In SC design problems, the objective can also be defined in terms of SC profitability, which considers the annual revenue and operating costs as well as the capital cost associated with the SC network. Different metrics, e.g., return on investment (ROI) and internal rate of return (IRR), can be used to estimate the long-term profitability of the SC.

3.1.4. Parameters

In an optimization framework, constant values are represented by parameters. They can be classified into the following categories:

- Cost data: Production costs, transportation costs, material handling costs, and transition costs are among the cost data used at the tactical and operational levels. The cost of establishing different facilities and processes is used, as well as the costs just mentioned, at the strategic level.
- Capacity data: Production capacity or production rate, warehouse capacity, and transportation rate are important capacity data used in an optimization framework. Some of these data represent the minimum and maximum capacities of various facilities, e.g., minimum and maximum production rate or minimum and maximum warehouse capacity.
- Production-related data: These data represent the efficiency of production lines, the quantity of materials consumed or produced, and conversion factors.
- Price data: These data represent the prices of feedstocks and materials as well as the prices of products in the optimization framework.
- Demand data: These data indicate the demand for each product in the market.

3.2. Executing the margins-based policy

As mentioned earlier in this chapter, what drives the margins-based policy is the ultimate profitability of the entire SC. All SC activities must be executed with respect to this policy. In the forestry industry, especially in the P&P sector, some SC practices are contrary to this approach. One of the most important of these practices is treating production cost as the major driver in decision-making. In this way, operating cost is generally used as the objective function, and the costs incurred by other nodes of the SC are basically neglected. Therefore, the first point to be made in an SC optimization framework with a margins-based policy is that profit must be used as the objective function.

Another common practice in the forestry industry is that products are produced in fixed known orders and sequences and the capability of the process for flexibililty in manufacturing and changeovers is not used. This can result in decreasing the profitability of the company when prices or demands change. Suppose that, based on the established sequences, the company has produced some products that in a particular period, are subject to low price or weak demand. In the case of weak demand, the company should store its products for a longer period, in which case the inventory cost rises. In such a case, the company might sell its products at a discount, which would decrease the profit. Moreover, some companies take orders based on their sequences, and they miss out on better orders just because these orders do not fit their production sequence. Hence, another point that must be respected in an SC optimization framework with a margins-based policy is to let the framework choose the best orders and to take advantage of the mill's capability of flexibility and changeover, leaving aside traditional recipes and practices.

4. Strategic SC design

In the strategic design of an SC, long-term decisions should be made. Such decisions include the type of products that should be produced, the technologies that should be used, the number, location and capacity of each type of facility, e.g., plants, warehouses and distribution centers, and the target markets. In a practical problem, it is difficult to address all these decision variables within a single SC optimization framework. Instead, it is preferable to pursue a systematic hierarchical methodology that addresses all these factors in a stepwise manner.

Because of the combinatorial aspect of such design problems, the hierarchical methodology might miss the global optimum. However, the methodology presented in this chapter does not seek to identify a global optimum. Rather, it seeks a set of feasible and practical biorefinery options (near-optimal solutions) that a company can strategically pursue. The decision as to what biorefinery strategy to take depends on many factors, most of which cannot be reflected in an optimization problem, e.g., understanding the market and market strategies, emerging products, processes, and technologies, the capabilities of existing SC assets, and potential partners. Many of these aspects can be addressed in different scenarios instead of being modeled into an optimization formulation. In this way, a simpler model will be solved, with more practical and realistic results.

Companies seek a set of biorefinery options that would significantly improve their business model. This should include the optimum and near-optimum solutions. This set of possible strategies should be pursued by a company in parallel with potential partners to establish mutual interests and to address most effectively the competitive disadvantages of forestry companies, such as lack of capital. This methodology would end up with a set of solutions. A multicriteria decision-making framework can be used to find the best option from a specific company's point of view, considering all the complexities involved in the industrial arena.

To achieve a stepwise methodology, some of these decisions must be made by integration with other methodologies. For instance, the set of products that should be produced can be determined by a product portfolio definition and selection methodology. The processes and technologies that should be used to produce the targeted products can be chosen through a technoeconomic study. The aspects that will be determined by the hierarchical methodology include:

(1) Flexibility design including the determination of the production capacity as well as the operating window as a design target, i.e., a range of production rates for each process, showing the flexibility capability of the plant and designing the production lines so that they can operate over the targeted range.

(2) SC network design, including determination of the number of facilities of each type, the location of each facility, and the capacity of warehouses and distribution centers, as well as partner selection. Note that network design-related decisions will be made through the generation of alternatives. These alternatives must be generated based on practical aspects of the problem that can be addressed in discussion with company experts and considering all features of the existing SC.

The methodology is illustrated in Figure 3. In the next section, the methodology will be explained using a hypothetical example. First, process design alternatives representing different levels of flexibility (volume flexibility) are defined. In the second step, which is independent of the first step, SC network alternatives are defined based on the assets of the existing SC and resources that are needed for new products. Then the process alternatives and the SC network alternatives are combined to create a set of process-SC network alternatives. Finally, using the SC optimization framework, the SC profitability of each combined alternative is calculated for different market scenarios. Thus, for each combined alternative, which represents a specific biorefinery with an implementation strategy, a set of SC profitability values for each market scenario is calculated. These profitability values will be used by experts to evaluate the various biorefinery options.

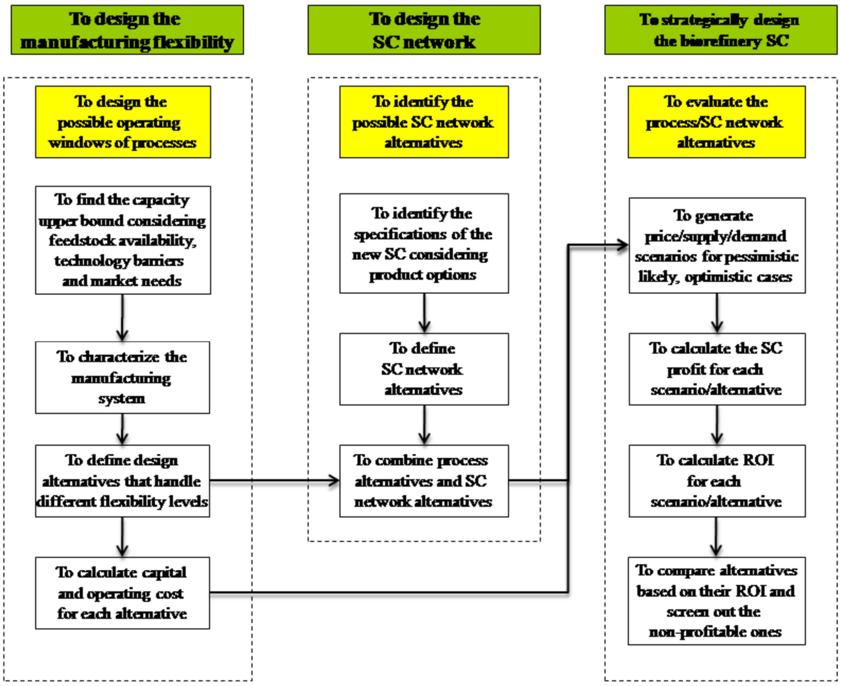

Figure 3. Hierarchical methodology for SC strategic design.

4.1. Design for flexibility

As discussed previously, product and volume flexibility are the most important dimensions of manufacturing flexibility in the FBR. Because the products that will be produced in the FBR plant are selected using the product portfolio definition methodology, the focus of this methodology is on designing for volume flexibility. Volume flexibility has two aspects: range of variations and speed of response, with the former being useful in the long term and the latter in the short term [45]. Therefore, at the strategic design level, the production capacity and the range of production rates, i.e., the operating window, must be designed for the long term to serve the short-term tactical and operational activities of the SC with the ultimate goal of SC profit maximization. At the short-term tactical-operational level, the designed flexibility should be exploited in a way that ensures that this ultimate goal will be reached. Therefore, SC-based analysis can be used to establish the range of production rates and to target an operating window which, when exploited against market volatility, would ultimately maximize SC profit.

In this methodology, establishing the design target for manufacturing flexibility is viewed through the SC operating philosophy. In other words, the range of production rates for each product is designed based on the SC profitability achieved by that design. Thus, what determines the design of manufacturing flexibility is the SC profitability resulting from the design.

Designing flexibility through SC optimization has not gained much attention. The holistic approach to designing and analyzing flexibility is to examine the tradeoff between the flexibility index and the cost of having flexibility. This cost includes either the cost of modifications needed for retrofit design or the cost associated with higher flexibility for a greenfield design. In the approach presented in this work, the cost is extended to the cost incurred by the activities performed over the entire SC. This implies taking into account not only the capital cost, but also all the SC operating costs incurred by designing for flexibility. In this way, SC cost and profitability are reflected at the design stage.

In the first part of the methodology, i.e., designing for flexibility, there are four steps: determining the upper bound for production capacity, characterizing the manufacturing system in terms of product and volume flexibility to recognize the modifications needed for the processes to become more flexible, generating design alternatives that can handle different production levels, and calculating capital investment and operating cost for each design alternative.

Illustrative example

To make the methodology more concrete, a hypothetical example is presented as an illustration. In this example, it is assumed that a P&P mill aims to implement FBR by producing bioproducts. Three product/process portfolios are considered and are shown in Table 2.

In the first portfolio, Fischer-Tropsch liquids (FTL) are produced by biomass gasification and a generic gas-to-liquid process, the products of which are separated into waxes and diesel. Finally, diesel is converted into jet fuel (JF). The second portfolio involves a series of fermenters. The majority of these are dedicated to butanol (BuOH) production, while the rest are used to produce succinic acid (SA) and lactic acid (LA). All three products are produced in similar fermenters, but each needs a specific recovery system. The third portfolio involves the family of four-carbon acids, i.e., succinic acid (SA), malic acid (MA), and fumaric acid (FA). They all can be produced and recovered on similar production lines.

Table 2. Price change scenarios.

Product portfolio No. 1	Product portfolio No. 2	Product portfolio No. 3
Fischer-Tropsch liquids (FTL)	Butanol (BuOH)	Succinic acid (SA)
Waxes and diesel	Succinic acid (SA)	Malic acid (MA)
Jet fuel (JF)	Lactic acid (LA)	Fumaric (FA)

4.1.1. Determining the capacity upper bound

To determine the operating window of each process, two steps are required: determining the maximum capacity, and determining the turn down ratio. The maximum possible capacities for each process are identified by considering three major factors: market demand, feedstock availability, and technological or technical barriers. On the other hand, to determine process turndown ratio, process design considerations must be addressed.

To determine the capacity upper bound, a basic technoeconomic study is carried out along with a simple market study. This combination considers market demand, feedstock availability, and technical barriers. After performing a market analysis to determine the market size and market share of the targeted products based on the available amount of feedstock, available technologies, and the possible production rates from a technical point of view as provided by the technology providers, as well as P&P process constraints and the integration strategy with biorefinery processes, a number of maximum-capacity options are identified. The term *possible production rate* refers to the maximum plant size that is technically feasible. This size is basically determined by the maximum size of one or more pieces of equipment in the process. This maximum size is often fixed by technical barriers, e.g., a piece of equipment cannot be built larger than a specific size, as well as restrictions on shipping the equipment to the plant site, e.g., a piece equipment larger than a specific size cannot be shipped on a railroad flatcar or truck [38].

In the case of a biorefinery implementation, feedstock availability is the most important factor in calculating the capacity upper bound. After investigating market size and market share of producers through the market study and identifying the maximum-capacity options, the availability of feedstock from different sources in and around the mill region is studied, and the cost of bringing the feedstock to the mill is estimated. Various factors should be taken into consideration in calculating the amount of available feedstock, e.g., price, proximity, seasonality, and transportation. Based on the results of feedstock availability and market demand studies, a number of the maximum-capacity options that were identified at the beginning of this step given the available technologies are chosen for further investigation.

Illustrative example

Figure 4 shows this step of the methodology for FTL. There are two maximum-capacity options identified for this product: 2000 t/d and 3000 t/d. Figure 4 shows the capital, operating, and transportation costs associated with these two options. It is apparent that the larger the capacity, the higher are the capital costs and the transportation costs, but the lower are the operating costs, because operating costs are calculated on a unit basis.

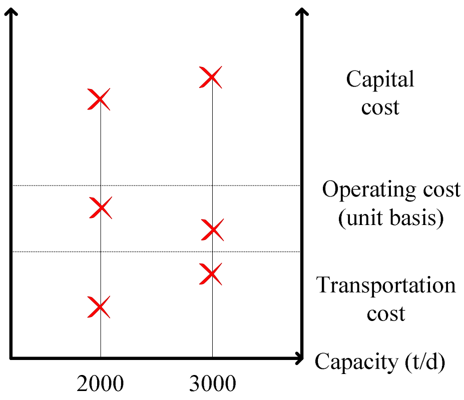

Figure 4. Capital, operating, and transportation costs for two technology options identified for FTL.

4.1.2. Characterizing the manufacturing system

It was previously stated in this chapter that manufacturing flexibility in the FBR involves four dimensions: feedstock flexibility, process flexibility, product flexibility, and volume flexibility. Feedstock and product flexibility are process-dependent attributes which are inherent in a process. In other words, a process must have the potential to accept different types of feedstock or to produce different products to be flexible. There are some processes that, by their nature, can accept only a specific type of feedstock or produce only one type of product and therefore cannot be designed to be flexible in these respects. As for product flexibility, Grossmann et al. in several studies [30,31,32] divided production systems into dedicated and flexible systems. Dedicated production systems operate in one mode and are used to produce one product, while flexible production systems can produce different products in different modes. Hence, processes can be either dedicated or flexible by their nature, and if a process does not have the potential for these two flexibilities, it cannot be designed to be flexible. However, process and volume flexibilities are attributes that are not process-dependent and can be designed into every process. Design for process and volume flexibility is basically part of early-stage design. Every process is designed in a way that can operate feasibly under changing conditions and over a range of production rates. The methodology presented in this chapter focuses on the volume-flexibility design for an FBR to enable it to be profitable under volatile market conditions. Note that the methodology does not deal with early-stage design, but considers the existing processes with their inherent flexibility and will retrofit the design in case the inherent flexibility is not sufficient to handle market volatility.

To design a flexible production system, this system must be characterized based on the following aspects:

- Process configuration: It should be verified whether the products can be produced in series, i.e., they are in one product family, such as diesel and jet fuel (Figure 5.a), or whether they should be produced in parallel lines because they are not from one family, for example, butanol and lactic acid (Figure 5.b).
- Product flexibility: It should be verified whether the system must be dedicated in terms of products, that is, with each production line producing a specific product (Figures 5.a and 5.b), or whether several products can be produced in a single line, for example if a line is able to produce more than one product in different production modes (Figure 6). An example of such products is succinic acid, malic acid, and fumaric acid. Using different reactor inputs, they can be produced in different modes of one batch system.
- Volume flexibility: It should be verified whether the process can handle a range of production rates. In other words, it should be determined whether the inherent flexibility of the process is enough or whether it must be made more flexible.

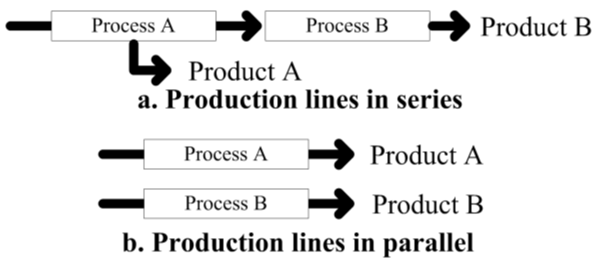

Figure 5. Separate production lines: a) in series, b) in parallel.

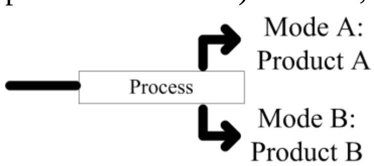

Figure 6. Flexible production line as defined by Sahinidis & Grossmann (1991).

To clarify how a manufacturing system can be characterized according to these aspects, the system presented by Yun et al. (2009) [41] will be used as a reference. They presented a biorefinery system which produces ethanol, lactic acid, itaconic acid, and citric acid. First, because these products do not belong to one product family, they cannot be produced in series, and separate production lines are needed. Second, all the acids can be produced in one line because the batch reactor is able to produce all of them in different modes based on the type of enzyme used in the process. A single recovery system can also be used to separate all three products from their coproducts. Therefore, only two parallel lines are needed, one for ethanol production and one for acid production. The third point is that the system can produce ethanol and lactic, itaconic, and citric acid in the ranges of 630–2100 kg/day, 872–1090 kg/day, 768–1100 kg/day, and 0–384 kg/day respectively. These production ranges can be used under different market conditions and, based on product price and market demand, products can be produced in different amounts. The process flow diagram of this system is shown in Figure 7.

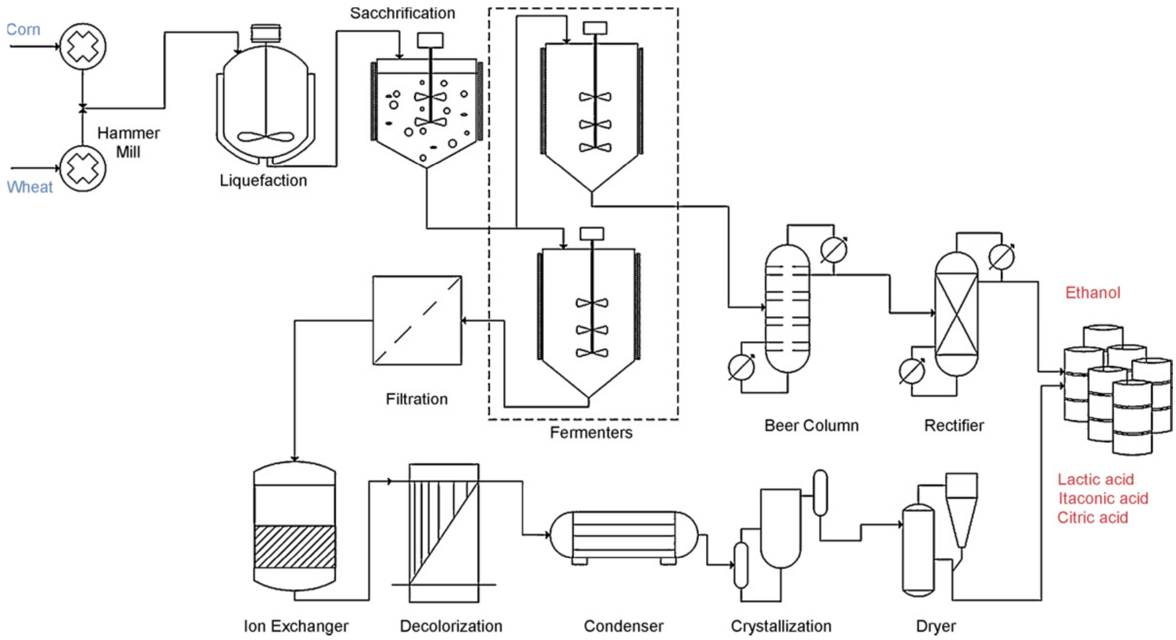

Figure 7. Process flow diagram presented by Yun et al. [41].

Illustrative example

The manufacturing processes in all three portfolios are characterized based on their defined characteristics as shown in Table 6. This characterization helps to define design alternatives representing different levels of flexibility in the next step.

Table 6. Process characteristics for each product/process portfolio.

Portfolio	Characteristics
FTL to waxes and diesel+ diesel to JF	Type of process: Continuous Process configuration: Lines in series Product flexibility: Each line produces only one product Volume flexibility: Each process has 10% turndown ratio
BuOH SA LA	Type of process: Batch Process configuration: Several lines in parallel Product flexibility: All products can be produced in similar fermenters, but in different modes. They need specific recovery systems Volume flexibility: Each process has 10% turndown ratio
SA MA FA	Type of process: Batch Process configuration: One line or several lines in parallel Product flexibility: All products can be produced in similar fermenters Volume flexibility: Each process has 10% turndown ratio

4.1.3. Defining design alternatives with different flexibility levels

Chemical processes are designed to operate at maximum capacity, which is generally called *nominal production rate*. Under changing conditions, whether for process-related or market-related reasons, the operating rate must be reduced to some extent. The distance (as a percentage of nominal rate) between the lowest point below the nominal production rate at which the process can efficiently operate and the designed nominal production rate is called the *turndown ratio*. The turndown ratio is a key concept in volume flexibility because it measures how flexible a process is in terms of throughput with respect to changing conditions. If these changes are in market price and demand, this process capability is of crucial importance. In a volatile market, it is desirable to produce products that are more profitable. Products are sold based on either long-term contractual demand or spot demand. Therefore, when producing a particular product is not profitable or is less profitable than producing another product based on the spot price, the plant should produce the more profitable product as much as it can while fulfilling contractual demands. If this amount is less than the amount that the plant can produce according to its nominal production rate, the production rate should be reduced. It would be desirable to use the extra capacity to produce another product, as is possible in batch processes if the production is scheduled properly. Sometimes the process has been designed in a way that it has the desired turndown ratio, that is, the turndown ratio is inherent in the design of the process. But if the inherent turndown ratio of the process is not sufficient, the process must be redesigned in way that can handle the required ratio. The goal of this section is to find the potential flexibility levels that can be achieved by doing retrofit design, and then to define design alternatives that can handle the defined flexibility levels.

Generally, there is one piece of equipment that limits the maximum and minimum capacity of a plant. Different pieces of equipment have flexibility in terms of their throughput and can operate within a range of operating rates. The maximum and minimum capacity of each piece of equipment can be calculated or be provided by the manufacturer. The minimum capacity of the piece of equipment which has the lowest minimum capacity will determine the maximum inherent turndown ratio of the entire process.

Sometimes it is desirable to have a greater turndown ratio than the inherent turndown ratio of the process. A simple way is to divide the production line, or the part of it that restricts the plant to a smaller turndown ratio, into smaller lines, so that if the production rate must be decreased, some of these smaller lines can be shut down. In this regard, the most important point is to know how the production line should be divided. In other words, the division ratio should be determined. The production line can be divided into two, three, or even more lines. Moreover, it can be divided in different ratios, i.e., 50–50, 70–30, 50–25–25, etc. Therefore, both the number of lines and the capacity of each should be defined.

This task is very much case-dependent. However, some hints can be helpful in making these decisions. The first hint is that the number of lines should not be very large. According to economies of scale, certain factors lead to a reduction in the average cost per unit as the scale of output or the size of a facility is increased. Therefore, one big reactor is less expensive than two smaller reactors with an aggregate capacity equal to that of the big reactor. Therefore, as the number of divisions rises, the capital investment and the operating cost will increase as well. Hence, the number and capacity of production lines should be determined so that the increase in capital and operating costs is compensated by the flexibility increase. The second hint is that small capacities should not be chosen for production lines. Assume a division of a production line with a capacity of 100 tons/day into two smaller lines. The possible ratios are 90–10, 80–20, 70–30, 60–40, and 50–50. The first two ratios are not appropriate options because they include small-capacity lines. Such small lines will be more expensive, on a per-unit basis, than bigger lines, again due to economies of scale. This will affect the return on investment. Moreover, in the case of flexible production lines which are able to produce more than one product, small lines may not be helpful because when they are changed over to produce another product, the amount produced on the small line may not be large enough to be able to respond to the customers.

Another strategy to make a system more flexible is to keep certain equipment or process sections on standby. This strategy will work for increasing capacity. The number of whatever piece of equipment restricts the process can be doubled so that when production increases, more capacity can be provided by the standby equipment. Again, the economic justification of adding a piece of equipment that will not be working all the time during plant operation is very important.

After determining the number and capacity of smaller production lines, the design alternatives must be defined in more detail. Each design alternative includes a new process configuration. The new configuration may need modifications the design of the pretreatment section, the heat exchanger network, or the separation and recovery system. In the case of flexible production lines, these modifications are of great importance. Products that are produced in a single production line might need different pretreatment and recovery processes. A batch system that is able to produce ethanol as well as acids needs different pretreatment and recovery systems for these two product families. Moreover, some products can be produced in different lines, but have some processing steps in common. For instance, biomass size processing and biomass drying areas might be similar for many processes, and therefore the important factors in their design would be their capacity and their linkage with other processing steps. Therefore, the number and capacity of all pretreatment and separation/recovery systems and the required links with all smaller lines should be considered in the design.

Illustrative example

Given the characteristics of each product/process portfolio in this illustrative example, different alternatives have been considered for each portfolio. Design alternatives representing different levels of flexibility for all portfolios are illustrated in Figure 8. The first portfolio, shown in Figure 8.a, includes three design alternatives. In the first alternative, A-1, FTL is separated into waxes and diesel. By changing the process conditions, the share of waxes and diesel can change from 45%–55% to 55%–45%. Therefore, there is some volume flexibility in the production of waxes and diesel. The waxes are sold, and 100% of the diesel is converted to jet fuel (JF) by a hydrotreating process. Another option would be to shut down the hydrotreating process and sell all the diesel to market. Moreover, the inherent volume flexibility of the hydrotreating process can be used to reduce the production of JF.

In the second alternative, A-2, a smaller hydrotreating process is used to convert diesel to JF. Hence, this system would be more flexible in terms of product. Again, the hydrotreating process can be shut down or its operating rate decreased to sell more diesel. The third alternative is the most flexible and is a combination of A-1 and A-2. Two small hydrotreating processes are used in parallel. If both are in operation, alternative A-1 is selected. If one of them is shut down, alternative A-2 is selected.

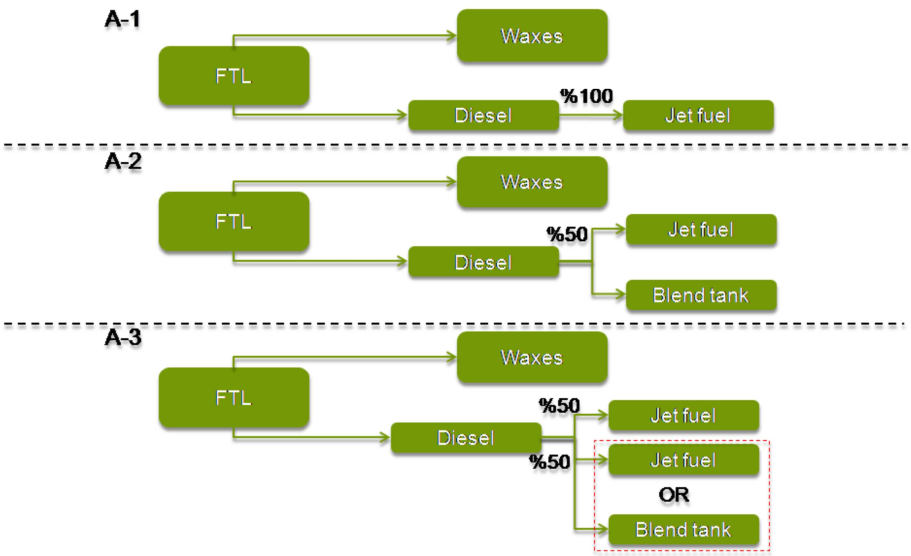

Figure 8.a. Design alternatives for portfolio 1.

For the second portfolio, two process alternatives have been considered, as can be observed in Figure 8.b. A series of fermenters in parallel are capable of producing different products based on their inputs. The majority of these are used to produce BuOH, while the rest are dedicated to SA and LA production. BuOH is a commodity with a large market, and therefore a fixed operating rate can be assigned to BuOH production, but SA and LA are more value-added, and flexibility would be useful in the production of these two products. Because the recovery system associated with each product is unique, or in other words, each recovery system can be used to recover only one specific product, this part of the process is the process bottleneck. In the first alternative, B-1, the inherent volume flexibility of each recovery system can be used to increase or decrease the production rate of each product. In the second alternative, a spare recovery system is used for SA and LA. These recovery systems are in standby mode. When it is decided, for instance, to reduce the production of SA and increase the production of LA, the fermenter is changed over to produce LA. The SA recovery system is shut down, and the spare LA recovery system will be put in operation to recover more LA.

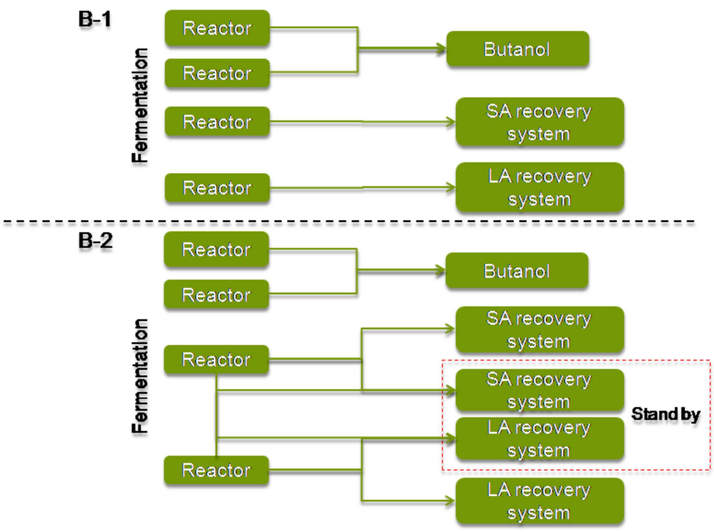

Figure 8.b. Design alternatives for portfolio 2.

For the third portfolio, two process alternatives have been considered and are illustrated in Figure 8.c. The family of four-carbon carboxylic acids, SA, malic acid (MA), and fumaric acid (FA), is produced. The production system is completely flexible, meaning that the system can produce all acids in different production modes based on the input to the fermenter. Moreover, all the acids can be recovered in a similar recovery system.

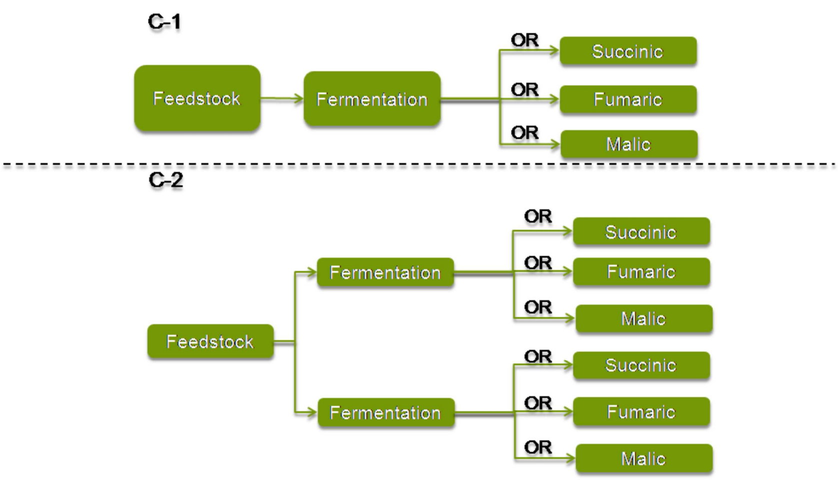

Figure 8.c. Design alternatives for portfolio 3.

The first alternative consists a single flexible production line which can be scheduled based on product price and demand. The production can be dedicated to the most profitable product among the three products. SC optimization can determine whether changeover to another product can be justified, that is, whether the changeover cost will be compensated and exceeded by the revenue gained from the production of the other product. This issue will be discussed in the last part of the methodology. The second alternative provides even more flexibility. Instead of having one production line, this alternative includes two smaller lines with an aggregate capacity similar to that of the first alternative. This alternative provides the opportunity of producing two out of three possible products at a time. Again, scheduling the production is complex, and optimization can help to find the best alignment between product price and demand on the one hand and production on the other.

4.1.4. Calculating capital and operating costs for each design alternative

In this step, the required capital investment for each design alternative and the major components of the operating cost associated with the nominal production rate are calculated. These costs will be used to estimate the profitability of each design alternative under different market scenarios.

The capital needed to purchase and install the required machinery and equipment, obtain the land, and to provide the service facilities, piping, and controls as well as the funds required for paying plant operational expenses before sales revenue becomes available is called the *total capital investment* (TCI). TCI consists of two components: *fixed capital investment* (FCI), which can be further divided into manufacturing fixed capital investment and nonmanufacturing fixed capital investment (also known as indirect cost), and *working capital* (WC) [45].

Manufacturing fixed capital investment includes the capital necessary for (a) purchasing equipment, (b) installing equipment, (c) instrumentation and controls, (d) piping and insulation, (e) electrical systems, (f) buildings associated with the process, e.g., substructures and superstructures, auxiliary buildings such as administration and office space, maintenance buildings such as electrical, piping, and building services including heating and dust collection, (g) yard improvements, (h) service facilities including utility facilities such as steam and water, water treatment, cooling towers, nonprocess equipment such as office, safety, and medical equipment, and distribution and packaging facilities such as raw material and product storage and handling equipment, and (i) the land.

Nonmanufacturing fixed capital investment or indirect costs represent construction overhead costs, including field office and supervision expenses, home office expenses, engineering expenses, miscellaneous construction costs, contractors' fees, and contingencies, plus costs associated with all plant components that are not directly related to the process operation, such as warehouses and laboratories.

The working capital is the total amount of money invested in raw material and supplies, finished products in stock, and semifinished products in the process, accounts receivable, cash kept on hand for monthly payment of operating expenses such as salaries, and finally accounts and taxes payable.

Calculating all these costs is complex. Hence, based on experience and rules of thumb, most of these costs can be estimated as a percentage of the total purchased equipment cost. Therefore, all components of direct costs, including purchased-equipment installation, instrumentation and control, piping, electrical systems, and buildings including services and yard improvements, can be estimated as a percentage of the major component of direct costs, *total purchased equipment cost* (TPEC). The sum of all these costs will give *total installed cost* (TIC), which is equivalent to direct cost.

Indirect costs can be estimated in the same way. All components of indirect costs, such as engineering and supervision, legal and contractors' fees, construction, and project contingencies can be related to the total purchased equipment cost (TPEC), the direct cost or total installed cost (TIC), or the total project investment (TPI), which is the sum of direct and indirect costs and is equivalent to fixed capital investment (FCI).

Working capital (WC) can also be considered as a function of total capital investment (TCI). WC as a percentage of TCI depends on the type of plant and generally varies from 10 to 20 percent. It might increase to 50 percent in some cases, especially for plants producing products with seasonal demand, as they need large inventories [45].

There are several ways to estimate the capital investment required for a plant. Peters et al. [46] introduces seven methods for this task: detailed-item, unit cost, percentage of delivered equipment cost, Lang factors for approximation of capital investment, power factor applied to plant/capacity ratio, investment cost per unit of capacity, and turnover ratio.

Another major component of an economic analysis is the aggregation of all costs related to plant operation, selling the products, recovering the capital investment, and contributing to corporate functions such as management and research and development. This component is called *total product cost* and can be subdivided into two categories; manufacturing or production or operating costs, and general expenses. Total product costs are generally calculated on a daily basis, a unit product basis, or an annual basis. Operating costs involves all expenses that are directly connected with plant operation. These expenses can be classified into three categories: variable production costs, fixed charges, and plant overhead costs. On the other hand, general expenses can be categorized into administrative expenses, distribution and marketing expenses, and research and development expenses. The focus in this step of the methodology is on the operating-cost calculation.

Variable operating costs consist of expenses directly related to the manufacturing operation, such as expenditures for raw materials, including transportation, unloading, etc., direct operating labor, supervisory and clerical labor directly related to the manufacturing operation, utilities, plant maintenance and repairs, operating supplies, laboratory supplies, royalties, catalysts, and solvents.

Fixed charges represent the expenses that are independent of production rate, such as expenditures for depreciation, property taxes, insurance, financing (loan interest), and rent.

Plant overhead costs cover expenses related to hospital and medical services, general plant maintenance and overhead, safety services, payroll overhead including social security and retirement plans, medical and life insurance, vacation allowances, packaging, restaurant and recreation facilities, salvage services, quality control laboratories, property protection, plant superintendence, warehouse and storage facilities, and special employee benefits.

Illustrative example

The capital investment required for each process in each portfolio is shown in Table 3. The more flexible an alternative is, the more capital investment it needs.

Table 3. Capital investment needed for design alternatives.

Portfolio 1		Portfolio 2		Portfolio 3	
Design Alter.	Cap. Inv. ($MM)	Design Alter.	Cap. Inv. ($M)	Design Alter.	Cap. Inv. ($MM)
A-1	180	B-1	56	C-1	43
A-2	110	B-2	65	C-2	47
A-3	195				

4.2. SC network design

In the strategic design of the SC network, decisions are made to design a new SC network or to redesign an already established SC network with all its existing assets. Such decisions involve the location of plants and determination of the target markets and the location and capacity of warehouses and transportation centers. The SC of a forestry company should be redesigned so that it can be used in the FBR. In the proposed methodology, the SC network design is performed in two steps. First, the specifications of the new SC are identified based on the characteristics of the new product options. Then SC network alternatives are defined. These SC network alternatives will be combined with the process design alternatives defined in the previous part of the methodology, and in the final part, SC optimization is used to calculate the SC profitability of each alternative.

4.2.1. Identifying the specifications of the new SC with product options

The SC networks of forest-products companies are in place with their own existing assets. Depending on the processes used in the mills, different facilities exist on the site. However, as mentioned previously, some processing steps are common among all processes in the mill, and therefore similar facilities and assets can be used or redesigned to be able to handle larger volumes.

Biomass receiving, processing, and storage areas in the mills generally include a biomass receiving and unloading station, biomass storage with a reclaimer, biomass processing involving a biomass size-reduction process, cleaning and wet storage, and finally biomass drying and dry storage. These facilities are used regardless of the fate of the biomass, i.e., the final product. Therefore, the design process should identify whether the new processes need the same facilities and whether the existing facilities have enough capacity for the larger amount of biomass that will be brought to the mill. If new or additional facilities are required, there is a need to investigate how those facilities should be modified or be added to the site to enable the mill to accept more biomass.

On the product side, the characteristics of new products must be taken into account to redesign the SC network. Each product has specific properties and characteristics which imply specific facilities for transportation and storage. Some products can be stored in warehouses, while others must be stored in tanks. Moreover, some products are transferred by truck or train, while others should be transported in a tanker or by pipeline. Therefore, the specifications of each product must be identified so that they can be addressed when defining SC network alternatives.

4.2.2. Defining SC network alternatives

With the existing SC assets and the characteristics of the products, the specifications of the new SC network can be identified. Based on these specifications, several SC network alternatives can be defined, which reflect the needs of the new SC network as well as the concerns of company experts. Several issues should be addressed when generating these alternatives;

- Partnership: Collaborating with other companies whose expertise brings value to the company’s business model must be considered in the SC network design. Partners can cooperate in producing a product, delivering the product, buying the product, and/or selling the product to the market. In this way, a part of the partner’s SC assets will be used, and less capital will be needed for establishing the new SC network.
- Location and capacity of distribution centers: based on the location of the plant, several target markets might exist in the areas around the plant. Therefore, different distribution centers with different capacities can be assigned to the target market areas. The role of partners in this issue is important. They might take the role of seller in the target markets, and they might have the required infrastructure for this purpose.
- Transportation network: Based on the characteristics of the products, different means of transportation can be used for product delivery. Again, partnerships can be used to reduce the capital costs required for establishing a transportation network. Contracts can be made with transportation companies which have a network of trucks or tankers and can simply deliver the products to the distribution centers. In addition, partners which buy the products or just deliver them to the market might have their own existing transportation network.

After defining SC network alternatives, the capital investment required to redesign the SC network based on each defined SC network alternative needs to be calculated. This capital investment should be added to the capital investment needed for the process design alternatives defined in the previous part of the methodology. This step will be discussed in the next section. The capital investment needed for the SC network alternatives which involve partnerships is smaller because a part of capital will be paid or has already been paid by the partner. However, it should be noted that the revenue will also be shared by the partner, and therefore less profit will be acquired by the company. The metric that can evaluate which strategy is better to pursue is the profitability of the entire SC, which takes into account both factors: capital investment reduction and revenue reduction. By calculating the profitability of each alternative, a tradeoff can be evaluated to unleash the value created by each strategy.

Illustrative example

Table 4 shows two SC network alternatives defined for the second portfolio.

Table 4. SC network alternatives for the second portfolio.

	SC network alternative for B-1	**SC network alternative for B-2**
Selling	BuOH: Contract with a blender SA: Partnership with a company LA: Partnership with a company	BuOH: Contract with a blender SA: Sell on the spot market LA: Sell on the spot market
Warehousing	Expand the existing warehouse Buy a new distribution center	Expand the existing warehouse
Transportation	Buy trucks to deliver the products to the customers	Contract with a transportation company to deliver the products

4.2.3. Combining process design alternatives and SC network alternatives

In this step, the process alternatives defined in the first part of the methodology are combined with the SC network alternatives defined in this part, so that the SC model can be run for each combined alternative in the next part. Each combined alternative will involve a process configuration with a specific level of flexibility for each product and an SC network related to those products. A total capital investment is associated with each combined alternative, which is the sum of capital investment required for the process alternatives and the capital investment needed for the SC network alternatives. It is of crucial importance to note that some facilities may be considered as either a part of a design alternative or a part of a SC network alternative. For instance, product storage is considered in the capital investment calculations. On the other hand, warehouse location and capacity determination is one of the major tasks performed in SC network design. Therefore, when defining the combined design/SC network alternatives, it is necessary to ensure that these SC nodes are not considered in both alternatives and that their associated capital investment is considered only once in the total capital investment for each combined alternative.

4.3. Evaluating the process design/SC network alternatives

The goal of this part of the methodology is to evaluate all defined process design/SC network alternatives from an SC perspective. The outcome of this part would be the profitability of each alternative under different market scenarios. This part contains four steps: first, a finite number of price/supply/demand scenarios, representing price and demand volatility, are generated. Then the SC profit for each alternative is calculated by SC optimization for each scenario. Then the profitability of each alternative is estimated for each scenario. Finally, the alternatives are compared based on their profitability, and the unprofitable ones are screened out.

4.3.1. Generating price/supply/demand scenarios

To address the uncertainty of market conditions and to reflect market volatility in the decision-making process, a scenario-based approach is used. Each scenario represents a specific market condition with respect to price, supply, and demand. Scenarios are generated in terms of feedstock supply, i.e., feedstock availability, and product demand, as well as feedstock and product prices. Scenarios must be generated to capture different market situations, that is, pessimistic, likely, and optimistic cases should be considered in scenario generation. Moreover, the relationships between supply, price, and demand should also be addressed during scenario generation. These relationships are highly complex and cannot be simplified into one holistic rule. They depend on whether the product is a commodity or specialty, price elasticity, policies, oil prices, and whether the product is a replacement product or a substitution product.

Another important factor in scenario generation is the time aspect. Scenarios can be generated for different time scales, and depending on the type of decisions to be made in the scenario analysis, scenarios can be generated for the short, medium, or long term. For strategic design-related decisions, scenarios should be generated for the long term, e.g., for a period of one year. As supply, demand, and price change during the year, the values associated with them can vary on a monthly or seasonal basis. Note that buying supply and selling products can be done based either on contracts or on the spot market. Contractual prices and demands imply fixed values during specific periods, meaning that the amount of product and its price in the contract can be fixed for the whole period of the contract or can change during certain periods based on the agreements reached at the time of making the contract, while spot prices are generally subject to changes based on the market situation. Therefore, both spot and contractual prices and demands must be addressed in scenario generation.

Illustrative example

In this step, scenarios are generated for one year. Scenarios are constructed for three cases: pessimistic, likely, and optimistic. For each case, only one scenario has been defined. Tables 5 and 6 show the contractual and spot prices and demands for the second portfolio. These scenarios represent price volatility and different demands in the market. In Table 5, the unit used for contractual demand is tons per year because the contracts are made for a period of one year. For the contracts, the price and the amount are fixed over the contract period. In Table 6, the unit of spot demand is tons per month. The prices can vary from month to month. For the sake of simplicity, an average monthly spot price has been shown for each product in Table 6. The first and third scenarios consider low price-weak demand and high price-strong demand for all products respectively, while the second scenario represents the most probable case in the market.

Table 5. Price and demand scenarios for contractual demands; in the demand column: P=pessimistic, L=likely, O=optimistic, C=contract.

Product	Pessimistic		Likely		Optimistic	
	Price ($/lb)	Demand (t/y)	Price ($/lb)	Demand (t/y)	Price ($/lb)	Demand (t/y)
BuOH	0.45	PCB	0.50	LCB	0.59	OCB
LA	0.58	PCL	0.64	LCL	0.71	OCL
SA	2.15	PCS	2.68	LCS	3.10	OCS

Table 6. Price and demand scenarios for spot demands; in the demand column: P=pessimistic, L=likely, O=optimistic, S=spot.

Product	Pessimistic		Likely		Optimistic	
	Price ($/lb)	Demand (t/y)	Price ($/lb)	Demand (t/y)	Price ($/lb)	Demand (t/y)
BuOH	0.40	PSB	0.55	LSB	0.69	OSB
LA	0.53	PSL	0.68	LSL	0.83	OSL
SA	1.95	PSS	2.73	LSS	3.30	OSS

4.3.2. Calculating the SC profit for each scenario/alternative

To evaluate design/SC network alternatives, the profitability of each alternative must be estimated. Therefore, the SC profit associated with each alternative in different market situations must first be calculated, and then, using the SC profit along with the capital investment, the profitability of each alternative can be estimated. The goal is to evaluate the performance of each alternative under different market conditions. Hence, in this step, the SC profit for each process design/SC alternative is calculated for every price/supply/demand scenario. To calculate the SC profit, the SC optimization model is used. The process configurations defined in the first part of the methodology as design alternatives, along with the SC network alternatives and the market scenarios generated in the previous step, are used as inputs to the model. The model optimizes SC profit by determining which orders to fulfill and calculating the optimum value of production rate related to each product and the flows of material between SC nodes. The overall problem at this stage can be stated as follows. Given:

- Number and length of time intervals
- Demand and price data for each feedstock, product, market, and time interval for each scenario
- Process configuration based on what was defined in the process design alternatives
- Configuration of the SC network based on what was defined in the SC network alternatives
- Capacity data of the nodes of the SC
- Direct cost parameters, i.e., unit production, transport, handling, and inventory costs based on operating cost calculations;

with the aim of profit maximization, find

- Orders to fulfill: which contracts to make, which spot demand to fulfill
- Production rates of each product for all time intervals and all market scenarios
- Flows of materials between the plants, warehouses, distribution centers, and markets
- SC profit.

Figure 10 shows this step graphically. The SC model is run for each design/SC network alternative for all market scenarios. The major output of the SC model is SC profit.

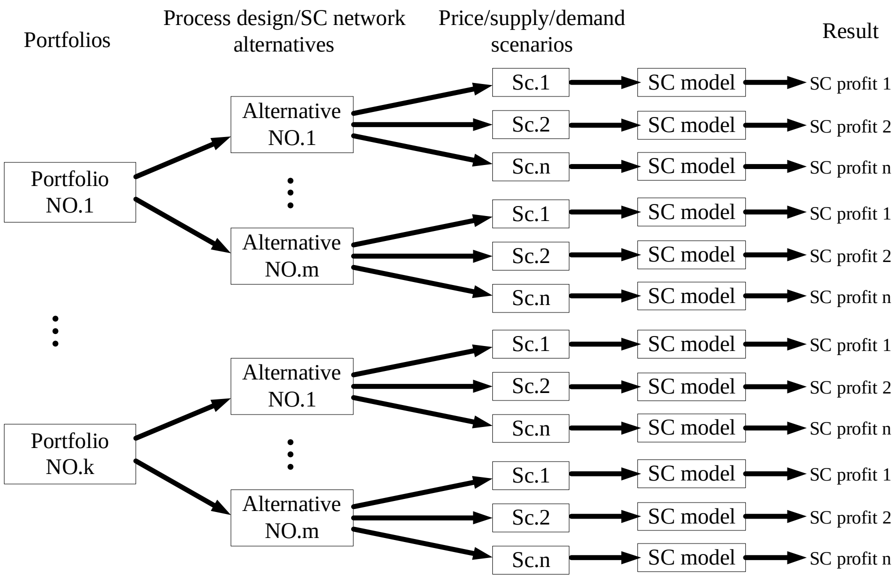

Figure 10. SC model inputs and outputs.

Illustrative example

Figure 11 demonstrates the results of this step graphically. The SC profit has been calculated for each design/SC network alternative for all market scenarios.

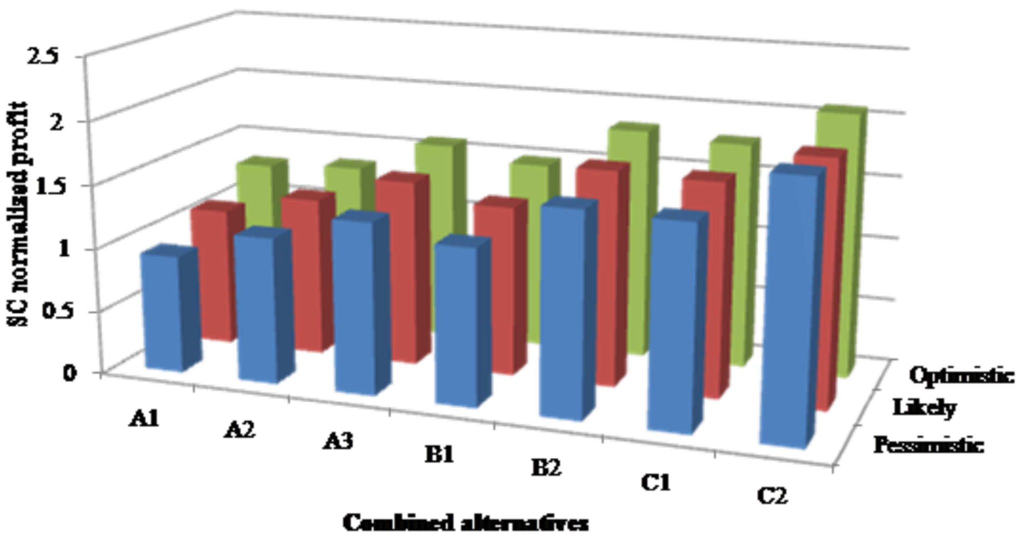

Figure 11. Normalized SC profit for each design/SC network alternative for all market scenarios.

4.3.3. Calculating the profitability of each scenario/alternative

To evaluate each process design/SC alternative, the profitability of each alternative should be estimated. There are several profitability estimation methods that can be used to estimate the profitability of a project. From a generic perspective, these methods can be divided into two main groups; methods that do not consider the time value of money, which include the rate of return on investment, payback return, and net return, and methods that consider the time value of money, which include the discounted cash flow rate of return and net present worth [45].

In this methodology, return on investment (ROI) is used as the measure of profitability. ROI is a simple measure which is generally used for preliminary design calculations. It does not consider the time value of money, variable depreciation allowance, increasing maintenance costs over the project life, or changing sales volumes [37]. However, because the proposed methodology involves a preliminary design study, ROI can be used as the profitability measure.

ROI is defined as the ratio of profit to investment. Any measure of profit and investment can be used in this ratio, but the most common measures are annual net profit and total capital investment. In this way, ROI would be the annual return on investment, which will be in the form of a fraction or percentage per year. Methods of estimating capital cost are introduced in Section 4.1.4. The net profit is calculated according to the following formula:

$$N_P = (s-c-d)\,(1-\Phi)$$

where N_P is the net profit after taxes, s is the revenue or the money earned from sales, c is the cost for operations, d is the depreciation charge, and Φ is the percentage of the gross profit that goes to income taxes. The revenue is generated by the sales of products produced by the plant. The annual revenue is the sum of the unit price of each product multiplied by its rate of sales. Depreciation is the amount of money (a part of the revenue) that is set aside to enable the company to replace equipment which wears out at the end of its lifetime. Generally, this amount of money is not used for this purpose, but instead it is invested in other ventures, and a part of the profits earned from the investment is used to replace the equipment. Governments specify the average lifetimes of different kinds of equipment. However, because there are various kinds of equipment in a plant, an average lifetime is considered for a specific plant. Depreciation can be computed by two methods: straight-line and ACRS, which are discussed briefly in Douglas [38].

For this step in the methodology, the net annual profit and capital investment are needed to calculate the ROI. Net annual profit was calculated in the previous step during SC profit maximization. The capital investment was estimated for each combined design/SC network alternative in Section 4.1.4. With these two components, the profitability of each combined alternative can be estimated for each market scenario.

Illustrative example

The results of this step are shown in Figure 12.

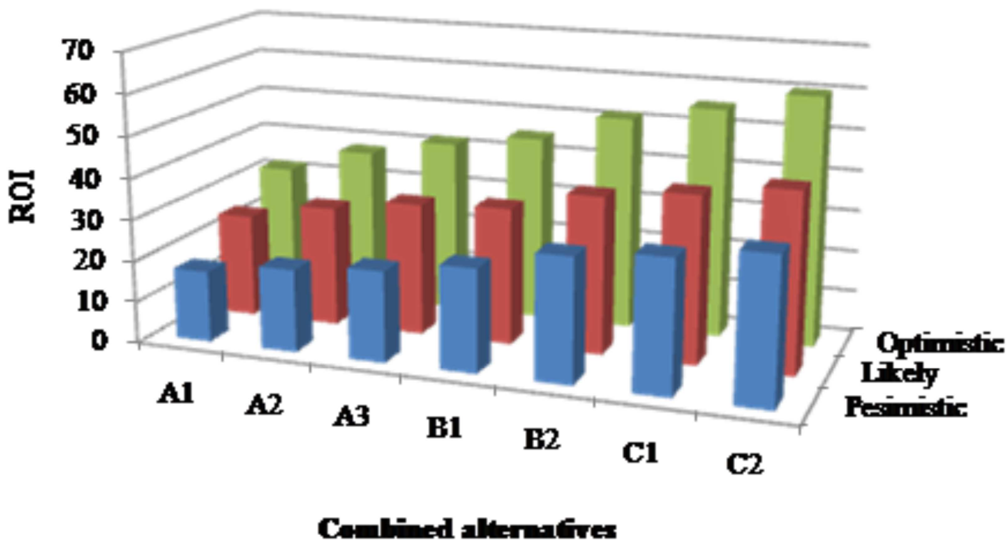

Figure 12. ROI for each design/SC network alternative for each market scenario.

4.3.4. Comparing the combined alternatives based on their profitability

The goal of this methodology is to evaluate the different biorefinery options that can be pursued by a company willing to implement the biorefinery. Each option involves a product/process portfolio, a process configuration with a specific level of flexibility, and an associated SC network. Each option must be analyzed from different perspectives, and the performance of the various options should be evaluated based on several metrics related to each perspective. The proposed methodology in this chapter looks at the options from a SC perspective and evaluates them based on their profitability, a concept that is then extended to SC costs and profitability. These options are analyzed by the proposed methodology, and their profitability is calculated. By comparing the profitability of alternatives and screening out the unprofitable ones, a set of biorefinery options that can be implemented by a company can be identified. The role of corporate executives in choosing the better options is a key factor. In fact, this methodology does not play the role of a decision-maker. Human knowledge and experience make the final decision; the proposed methodology simply serves this decision-making process.

Finally, it should be mentioned that an implementation strategy can also be defined for each option by defining process design/SC network alternatives. Companies often think about implementing the biorefinery through an incremental strategy. They might plan to start their biorefinery project by producing some commodity products and then, after several years, adding more processes to their portfolio to produce more value-added products from commodities. This strategy can be considered in the proposed methodology. The design/SC network alternatives can be defined in a way that reflects the incremental aspect of biorefinery implementation. Each alternative should be divided into a set of time frames, and for each time frame, a specific process configuration and a specific SC network should be defined according to the implementation strategy proposed by the company. In the first time frame of the alternatives, the process configuration and SC network related to the first set of products are defined, and in the following time frames, the necessary changes and additions which should be made to both the processes and the SC network are added. However, to apply the methodology for this purpose, some of its steps must be modified. Capital investment should be estimated by methods which consider the time value of money, design alternatives must take into account the future evolution of technology, partnerships and contracts with other companies should consider the implementation plan, and supply, demand, and price in future markets must be better forecasted.

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APPENDIX J – Conference Paper: Metrics for evaluating the forest biorefinery supply chain performance

Metrics for Evaluating the Forest Biorefinery Supply Chain Performance

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Abstract

The forest biorefinery (FBR) is emerging as a possibility for improving the business model of forest product companies, however introduces significant challenges in terms of market, technological, and financial risks - which can be addressed to an important extent in the design of supply chains (SC). For sustainable decision-making regarding biorefinery strategies, criteria from different perspectives, i.e. economic, environmental and social, should be considered. The economic criteria that are used for decision making typically do not consider volatility, whereas today's market is subject to volatilities in terms of price and demand. It is critical that biorefinery strategies are flexible in order to be robust to market volatility. This paper presents metrics of flexibility and robustness, showing the performance of the SC in a dynamic environment. These metrics are suitable to be used in a multi-criteria decision-making (MCDM) framework for the evaluation of the FBR SC strategies. Moreover, a "conditional value-at-risk" parameter is introduced for analyzing levels of risks in making market-related decisions.

Keywords: Forest Biorefinery, Supply Chain, Flexibility, Robustness, Value-at-risk

1. Introduction

FBR is increasingly considered as a possibility for improving the forest products company business model, though it poses market, technological, and financial challenges. Thus, potential FBR implementation strategies must be analyzed using different perspectives to identify the most promising ones [1]. Sustainable development includes three dimensions; economic,

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environmental, and social. MCDM frameworks can consider several metrics provided from different analysis tools to permit the analysis of different strategies [2]. Hence, MCDMs can be used for sustainability analysis, if appropriate metrics for economic, environmental and social aspects of a strategy can be assessed.

Economic metrics that are used in decision making, which are mainly related to the profitability of a strategy, are incapable of accounting for the market volatility [3]. Sensitivity analysis is typically executed to address the impact of possible market scenarios on profitability. Even in this case, the problem is viewed as a steady-state case and the dynamism of the market, i.e. changes in price and demand over the given time period, are ignored. Moreover, it is not easy to use the result of a sensitivity analysis in an MCDM framework. Instead, it is desirable to reflect the response of a strategy to such dynamism by relevant metrics. This paper presents metrics of flexibility and robustness that can be used in an MCDM framework, in conjunction with economic criteria, for the evaluation of the FBR SC strategies. These metrics are the outcomes of an analysis that evaluates the impacts of the SC design on operational SC activities.

2. Problem statement

The decisions as to which products to produce, which technologies to employ, with which companies to make partnerships, and which parts of the SC to redesign are major strategic decisions addressed by a forest product company implementing the FBR. The SC of an FBR must be designed to be flexible, so that it can have a robust response to market volatility. The goal of this paper is to evaluate the performance of several FBR design options using metrics of flexibility and robustness. Design options with different levels of flexibility in production and with different SC networks are considered, and their performance in case of several market scenarios is tested. An SC optimization model calculates the profit of design options for every market scenario and quantifies the flexibility and robustness of each option using the introduced metrics. These metrics can be further used in an MCDM framework along with metrics provided by other tools, e.g. life cycle analysis (LCA), to identify the best option. Finally, a conditional value-at-risk parameter is introduced to analyze levels of risk in making market-related decisions and to provide required information for profit-risk trade-offs.

3. Performance metrics

3.1. *Manufacturing flexibility: Metric of flexibility (MF)*

Today's market is subject to huge volatilities in terms of price and demand. An FBR will be exposed to this kind of volatile environment and hence, flexibility, of any possible type, must be exploited in an FBR to mitigate risks. An FBR will be able to produce several products, including P&P products, bioproducts, and energy. Producing several products implies the opportunity to take advantage of manufacturing flexibility, i.e., producing different products (product flexibility) at different volumes (volume flexibility) in different time periods. In a volatile market, depending on feedstock and product prices as well as supply and demand, manufacturing flexibility can be exploited, and the mill can produce different products in different amounts to optimize the profit.

To quantify the volume flexibility, MF shown in equation 1, inspired by [4], is introduced:

$$MF = \sum_t \sum_p \sum_m \left(\frac{C_{mpt} - C_{mp}^N}{C_{mp}^N}\right) \quad (1)$$

where C_{mpt} is the amount of product *m* that is produced on process *p* in time period *t* and C_{mp}^N is the amount of product *m* produced on process *p* by the nominal production rate over the same number of processing hours.

3.2. *Robustness: Metric of robustness (MR)*

In a robust design the control parameters of a system are selected in such a way that the desirable measured function do not diverge significantly from a given value [5]. Several robustness metrics have been introduced thus far [6]. Well-known metrics are standard deviation and mean absolute deviation. For the sake of simplicity and interpretability for an MCDM panel, we use a simple formulation as robustness metric, as shown in equation 2.

$$MR = \left(\frac{\sum_{Sc}(Pr_B - Pr_{Sc})}{Pr_B}\right)^{-1} \qquad (2)$$

where Pr_B is the base case profit, Pr_{Sc} is the profit for scenario *Sc* and N_{Sc} is the number of scenarios. To quantify the downside risk of volatility, scenario profits that are less than the base case profit are considered in this equation.

3.3. *Conditional value-at-risk (CVAR)*

As discussed by Verderame and Floudas [7], CVAR aims at guarding against realization of uncertain parameters by going beyond the expected evaluation when expressing the uncertainty of system parameters. A loss function must be defined as a function of decision vector and uncertain parameters with a probability distribution. Using the loss function and the acceptable loss level, two constraints are added to the optimization formulation which restrict the evaluation of the system's variables according to a user-specified risk aversion parameter.

Inspired by [7], a constraint is added to the optimization formulation, in which the contractual order acceptance percentage (OA) should be bigger than a risk factor. A high OA implies less risk, because contractual orders are fixed in price and amount over the long term and thus they can secure the profit. On the other hand, lower OA connotes more spot orders which might cause profit increase, but poses higher risks, as spot demands are not certain. The added constraint is shown in equation 3:

$$\frac{\text{Volume associated with the accepted contractual orders}}{\text{Volume associated with all contractual orders}} > \alpha \quad (3)$$

where α is the risk parameter. Probability of market scenarios has not been considered in this study.

3.4. *SC optimization framework*

The SC model aims at maximizing SC profit. Inspired by the tactical model developed for the chemical industry presented in [8], this model considers the management of a multi-product, multi-echelon SC, including production facilities, inventories and a number of customer zones. Feedstock is provided by several suppliers. Processes are either dedicated or flexible, i.e. they are able to produce several products through different recipes. Changing from one recipe to another incurs changeover cost and time. The steam required for each process is provided by both fuel and biomass. Inventories can receive material from different sources and plants, and supply different markets. Each market places demand in two ways: by contract, i.e., for the long term, and on the spot, i.e., for the short term. In case of a contract, specific quantities of products must be sold to the customer in specific time periods. The spot demand can be partially fulfilled. Transportation routes link suppliers, facilities and customers together. The model is formulated as an MILP with a discrete time horizon of 52 weeks. The model exploits the potential for flexibility and determines which orders must be fulfilled, how much of which products must be produced, stored, and delivered to the market.

4. Results and discussion

A simplified example, including two biorefinery design options, is presented, as shown in figure 1. In option B-1, there are two parallel lines, including a fermentor, which is flexible, and a recovery system. One line produces lactic acid (LA) and the other line is able to produce both succinic acid (SA) and malic acid (MA), as one recovery system can be used for both products. To increase the level of flexibility, a new SA/LA recovery system is added in option B-2 so that the first line can produce all three products. Based on the market conditions, the fermentor produces one of the products and the relevant recovery system is used, while the other recovery system will be out of operation. The SC optimization is run for nine market scenarios, and profit, flexibility and robustness metrics of each design is calculated.

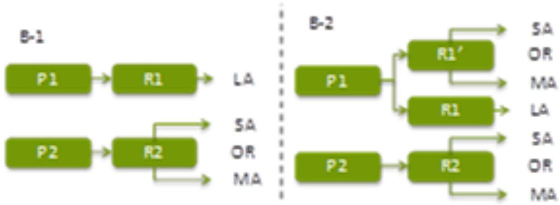
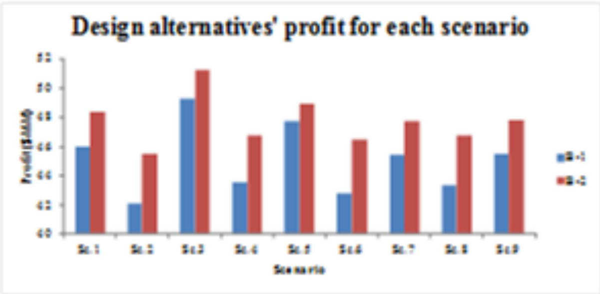


Figure 1. Design options

Table 1 shows the calculated profit and flexibility of both options for each market scenario. The flexibility metric for the second option, which has more potential for flexibility, is higher for all scenarios. Profit is also higher for the more flexible option and that shows more flexibility results in more profit. Using average profit, a simple return on investment (ROI) was estimated, which shows the more flexible option has a higher ROI. Thus, although extra capital should be spent on more flexible option, this extra capital is well compensated by the increase in flexibility. Finally, robustness metric shows that the more flexible option is more robust against market volatility and the deviation of profits from the base case profit is less than that of the less flexible option. The results are shown graphically in figures 2 and 3.

		Sc.1	Sc.2	Sc.3	Sc.4	Sc.5	Sc.6	Sc.7	Sc.8	Sc.9	Avg.Profit	ROI	MF	MR
B-1	Profit ($MM)	46	42	49	43	47	42	45	43	45	45	43%	25%	3.4
	Flexibility	25%	24%	29%	23%	27%	25%	25%	26%	23%				
B-2	Profit ($MM)	48	45	51	46	48	46	47	46	47	47	45%	30%	5.2
	Flexibility	32%	27%	35%	27%	32%	26.%	33%	26%	33%				

Table 1. Profit, ROI, flexibility and robustness of design options



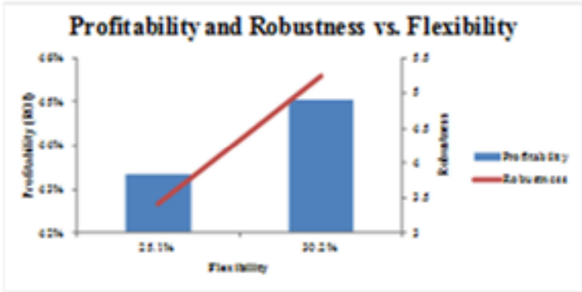


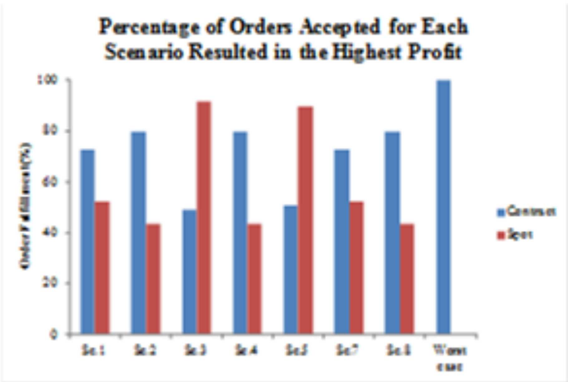
Figure 2. Profit of options for market scenarios   Figure 3. Robustness vs. Flexibility

Table 2 shows the result of CVAR studies for option B-1. SC model was run for eight market scenarios and the profit was calculated for several levels of OA. The maximum profit happens in different percentages (highlighted in yellow), showing that there is not one optimum percentage for all scenarios. In 80% OA, the average profit is the highest and the robustness metric is the lowest, except compared to the 100% OA which has a low profit, but the best robustness. Therefore, 80% OA can be chosen over lower OAs and compared to 100% OA. Decision makers with low risk tolerance may choose 100% OA which has better robustness, while those with higher risk tolerance can choose 80% OA which has the highest profit.

OA%	Sc.1	Sc.2	Sc.3	Sc.4	Sc.5	Sc.7	Sc.8	Worst	MR	Profit
22.03%	37.57	34.16	40.32	34.33	38.27	37.47	34.25	7.66	0.93	33.01
28.81%	39.52	36.11	42.27	36.28	40.22	39.43	36.21	9.28	0.98	34.92
49.15%	45.08	42.08	**47.77**	42.25	45.86	44.98	42.17	16.33	1.19	40.82
50.85%	45.16	42.29	47.77	42.46	**45.92**	45.06	42.38	16.87	1.22	40.99
72.88%	**45.19**	44.36	45.97	44.53	44.43	**45.09**	44.46	24.16	1.93	42.28
79.66%	45.17	**44.80**	45.52	**44.97**	44.28	45.07	**44.90**	25.95	**2.24**	**42.59**
100.00%	35.94	35.35	38.33	35.35	36.12	35.94	35.35	**34.00**	**9.74**	**35.80**

Table 2. Profit, robustness and average profit for option B-1

Figure 4 and 5 show the results graphically. For the optimistic scenarios (3 and 5), the maximum profit happens in lower OAs compared to other scenarios, because in these scenarios the spot market is strong and more spot orders are accepted and lower OA results in higher profit. By contrast, for pessimistic scenarios (2 and 4), more contracts are accepted, because the spot market is weak. For the worst case scenario (8), the maximum profit is acquired at 100% OA, because the spot market is not profitable at all and at 100% OA, where all contracts are made, the profit is maximized.



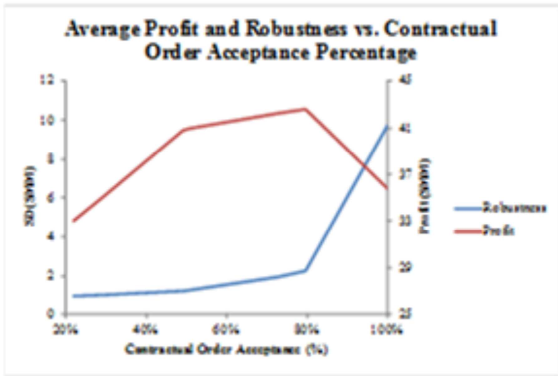


Figure 4. OA for spot and contractual orders   Figure 5. Profit and robustness vs. OA

5. Concluding remarks

To mitigate the risks of market volatility, the processes and the SC must be designed flexible to have a robust response to changing market. Although more flexible design alternatives are more capital intensive, the results show that this capital will be very well paid off by increasing the capability of the system to react properly to market changes and a more flexible alternative will be more profitable and robust. Moreover, the CVAR studies show that optimum OA is different for each market scenario. This study demonstrates that lower risks may imply lower profit and thus, an appropriate trade-off analysis ought to be performed to choose the right OA.

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